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Supporting Information

Epoxy Isonitriles, A Unique Class of Antibiotics: Synthesis of Their Metabolites and Biological Investigations

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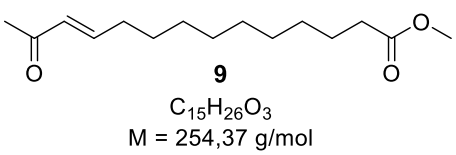
1. Synthesis

1.1. Instrumentation and General Notes

NMR spectra were recorded using the following spectrometers: INOVA (600/150 MHz), INOVA (500/125 MHz), Bruker Ascend (600/150 MHz), INOVA (400/100 MHz), or VNMR (400/100 MHz). Chemical shifts are quoted in ppm relative to tetramethylsilane and with the indicated solvent as an internal reference. The following abbreviations are used to describe signal multiplicities: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad), dd (doublet of doublets), dt (doublet of triplets), etc. Accurate mass spectra were recorded on a Thermo LTQ-FTMS APCI or ESI as indicated. Specific rotation measurements were made with a 1 dm path length using a Perkin Elmer 341 Polarimeter. Non-aqueous reactions were performed under an atmosphere of argon, in flame-dried glassware, with HPLC-grade solvents purified on a Pure Process Technology purification system. Amine bases were freshly distilled from CaH_2 prior to use. Brine refers to a saturated aqueous solution of sodium chloride. "Column chromatography", unless otherwise indicated, refers to purification on a Biotage Isolera One Automated system in a gradient of ethyl acetate in hexanes, or by standard flash chromatography techniques on small scale (<100 mg). Reactions were monitored via thin-layer chromatography (TLC) using EMD Millipore® TLC silica gel glass plates with $KMnO_4$ or vanillin stain.

1.2. Synthesis of *post*-aerocyanidin (+)-**4**

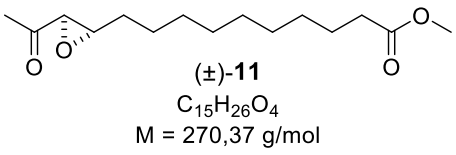
Methyl (*E*)-13-oxotetradec-11-enoate (9). In a flame dried flask equipped with a metal stir bar were added alkene **7** (1.50 g, 7.06 mmol, 1 equiv) in diethyl ether (0.5M), methyl vinyl ketone (1.75 mL, 21.0 mmol, 3 equiv), Grubbs Catalyst, 2nd Generation (120 mg, 0.141 mmol, 2 mol %), and CuI (40 mg, 0.21 mmol, 3 mol %). The solution was stirred under argon at room temperature overnight, quenched with a saturated aqueous solution of ammonium chloride and extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over anhydrous magnesium sulfate, and concentrated *in vacuo*. The resulting yellow residue was purified *via* column chromatography to afford **9** as a slightly yellow oil (1.66 g, 92% yield).



9
$C_{15}H_{26}O_3$
M = 254,37 g/mol

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.79 (dt, J = 15.9, 6.9 Hz, 1H), 6.06 (dt, J = 15.9, 1.5 Hz, 1H), 3.66 (s, 3H), 2.29 (t, J = 7.5 Hz, 2H), 2.24 (s, 3H), 2.23–2.17 (m, 2H), 1.65–1.55 (m, 2H), 1.50–1.39 (m, 2H), 1.27 (s, 10H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.6, 174.2, 148.5, 131.2, 51.3, 34.0, 32.4, 29.23 (2C), 29.14, 29.08, 29.03, 28.0, 26.7, 24.8; **HRMS** ESI (*m/z*) calcd for $C_{15}H_{27}O_3$ [M+H$^+$]: 255.19547, found 255.19554.

Methyl 10-((2*S,3*R**)-3-acetyloxiran-2-yl)decanoate ((±)-11).** To a stirred solution of alkene **9** (860 mg, 3.38 mmol, 1 equiv) and *tert*-butylamine (4 µL, 0.034 mmol, 1 mol %) in methanol (27 mL) at 0 ˚C were slowly added 30% by weight hydrogen peroxide (1.9 mL, 13.5 mmol, 4 equiv). The solution was allowed to warm to room temperature and stirred overnight. The reaction was quenched with a 1:1 mixture of saturated sodium thiosulfate and sodium bicarbonate and extracted with three portions of dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The resulting oil was purified *via* column chromatography to afford epoxide (±)-**11** as a colorless oil (672 mg, 74% yield).

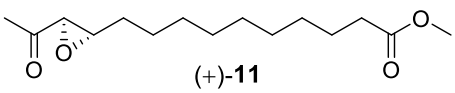


(±)-**11**
$C_{15}H_{26}O_4$
M = 270,37 g/mol

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.66 (s, 3H), 3.17 (d, J = 1.9 Hz, 1H), 3.08–3.04 (m, 1H), 2.29 (t, J = 7.5 Hz, 2H), 2.05 (s, 3H), 1.68–1.53 (m, 2H), 1.51–1.38 (m, 2H), 1.37–1.20 (m, 12H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 206.3, 174.4, 60.1, 58.2, 51.6, 34.2, 31.9, 29.48, 29.38, 29.33, 29.31, 29.22, 25.9, 25.0, 24.5; **HRMS** ESI (*m/z*) calcd for $C_{15}H_{27}O_4$ [M+H$^+$]: 271.19039, found 271.19049.

Methyl 10-((2*S*,3*R*)-3-acetyloxiran-2-yl)decanoate ((+)-11). 9-amino-*epi*-Quinidine (97 mg, 0.15 mmol, 30 mol %) was added to a solution of trifluoroacetic acid (57 µL, 0.75 mmol, 1.5 equiv) in 1 mL of dioxane (0.25M). Alkene **9** (127 mg, 0.5 mmol, 1 equiv) was added and the solution was stirred at 50 ˚C. After 15 minutes, 30% by weight sodium hydroxide (0.1 mL, 0.6 mmol, 1.5 equiv) were added and the solution was stirred overnight. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. To the resulting white solid were added 2 mL anhydrous methanol and 1 M solution of sodium methoxide in methanol (0.5 mL, 0.5 mmol, 1 equiv). After two hours, the reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc.

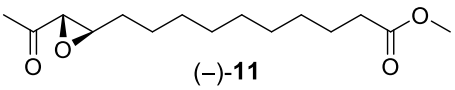
The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. Purification was performed by column chromatography resulting in epoxide (+)-**11** as a low-melting point white solid (73.5 mg, 54% yield).



(+)-**11**
$C_{15}H_{26}O_4$
M = 270,37 g/mol

$[\alpha]_D^{20}$ +27.3 (*c* 0.73, $CHCl_3$).

Methyl 10-((2*S*,3*R*)-3-acetyloxiran-2-yl)decanoate ((–)-11). 9-amino-*epi*-Quinine (97 mg, 0.15 mmol, 30 mol %) was added to a solution of trifluoroacetic acid (57 µL, 0.75 mmol, 1.5 equiv) in 1 mL of dioxane (0.25M). Alkene **9** (127 mg, 0.5 mmol, 1 equiv) was added and the solution was stirred at 50 ˚C. After 15 minutes, 30% by weight sodium hydroxide (0.1 mL, 0.6 mmol, 1.5 equiv) were added and the solution was stirred overnight. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. To the resulting white solid were added 2 mL anhydrous methanol and 1 M solution of sodium methoxide in methanol (0.5 mL, 0.5 mmol, 1 equiv). After two hours, the reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. Purification was performed by column chromatography resulting in epoxide (–)-**11** as a low-melting point white solid (74.5 mg, 55% yield).

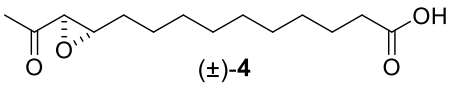


(–)-**11**
$C_{15}H_{26}O_4$
M = 270,37 g/mol

$[\alpha]_D^{20}$ –26.6 (*c* 1.58, $CHCl_3$).

10-((2*S,3*R**)-3-Acetyloxiran-2-yl)decanoic acid ((±)-4).** To a stirred solution of methyl ester (±)-**11** (10 mg, 0.037 mmol) in THF/H_2O (1:1, 1 mL) at 0 °C was added LiOH (2.7 mg, 0.11 mmol, 3 equiv). The reaction was warmed to room temperature and stirred for one hour. The reaction was quenched with a 1M aqueous solution of HCl and extracted with CH_2Cl_2. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The residue was purified by flash chromatography to afford the product (±)-**4** as a colorless oil which solidify in the fridge (7.0 mg, 74% yield).

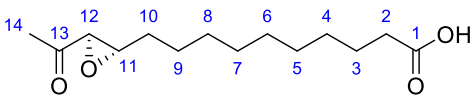
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (d, J = 2.0 Hz, 1H), 3.07 (ddd, J = 6.1, 5.0, 2.0 Hz, 1H), 2.35 (t, J = 7.5 Hz, 2H), 2.06 (s, 3H), 1.70–1.54 (m, 2H), 1.53–1.38 (m, 2H), 1.38–1.21 (m,



(±)-**4**
$C_{14}H_{24}O_4$
M = 256,34 g/mol

12H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 206.4, 179.2, 60.1, 58.2, 34.0, 31.9, 29.47, 29.36, 29.32, 29.28, 29.14, 25.9, 24.8, 24.5; **HRMS** ESI (*m/z*) calcd for $C_{14}H_{25}O_4$ [M+H$^+$]: 257.17474, found 257.17475.

10-((2*S*,3*R*)-3-Acetyloxiran-2-yl)decanoic acid ((+)-4). To a stirred solution of methyl ester (+)-**11** (12 mg, 0.044 mmol) in THF/H_2O (1:1, 1 mL) at 0 °C was added LiOH (3.3 mg, 0.13 mmol, 3 equiv). The reaction was warmed to room temperature and stirred for one hour. The reaction was quenched with a 1M aqueous solution of HCl and extracted with CH_2Cl_2. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The residue was purified by flash chromatography to afford the product (+)-**4** as a colorless oil which solidify in the fridge (5.5 mg, 49% yield).



(+)-**4**
$C_{14}H_{24}O_4$
M = 256,34 g/mol

[α]$_D^{20}$ +12.2 (*c* 0.32, MeOH);
[α]$_D^{20}$ +11.0 (*c* 0.30, MeOH, litt)[1]

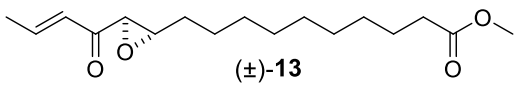
Supplementary Table S1. Comparison of ^{1}H and ^{13}C NMR spectra of (+)-**4** and the natural product ($CDCl_3$).

	δ_H			δ_C	
	Natural (400 MHz)	**Synthetic (600 MHz)**		**Natural**	**Synthetic (600 MHz)**
1	-	-		-[a]	179.2
2	2.35, t (7.5)	2.35, t (7.5)			34.0
3	-[a]	1.70–1.21			31.9–24.8
4					
5					
6					
7					
8					
9					
10					
11	3.07, ddd (6.0, 5.0, 2.1)	3.07, ddd (6.1, 5.0, 2.0)			58.2
12	3.18, d (1.8)	3.18, d (2.0)			60.1
13	-	-			206.4
14	2.06, s	2.06, s			24.5

[a] Not reported

[1] Parker, W. L.; Rathnum, M. L.; Johnson, J. H.; Wells, J. S.; Principe, P. A.; Sykes, R. B. (1988) Aerocyanidin, a New Antibiotic Produced by *Chromobacterium Violaceum*. *J. Antibiot. 41* (4), 454–460.

Methyl 10-((2*S,3*R**)-3-((*E*)-but-2-enoyl)oxiran-2-yl)decanoate ((±)-13).** To a stirred white suspension of methylketone (±)-**11** (111 mg, 0.41 mmol, 1 equiv) in THF (5 mL) at –78 °C was added LiHMDS (460 µL, 1M in THF, 0.46 mmol, 1.5 equiv). After 30 min, acetaldehyde (69 µL, 1.23 mmol, 3 equiv) was added to the clear slightly yellow solution and the reaction mixture was stirred for 1 h at this temperature. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The crude residue was filter through a plug of silica and eluted with a mixture of Hexanes/EtOAc (1:1). The residue was then purified by a plug of silica gel, eluting with 50% EtOAc/hexanes, to give the corresponding mixture of alcohols, which was taken for the next step without further characterization. Analysis of the residue by ^{1}H NMR spectroscopy *indicated the formation of a 1:1 mixture of both diastereomers*. To a solution of the residue in CH_2Cl_2 (3 mL) was subsequently added Et_3N (166 µL, 1.23 mmol, 3 equiv) and MsCl (48 µL, 0.62 mmol, 1.5 equiv) at 0 °C. The reaction was then warmed to room temperature and stirred for 1h. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The crude residue was purified by flash chromatography to afford the product (±)-**13** as a colorless oil (76.0 mg, 63% yield).

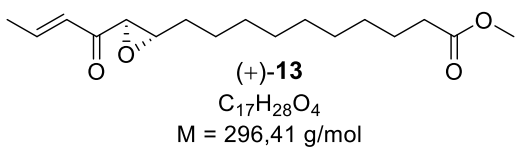


(±)-**13**
$C_{17}H_{28}O_4$
M = 296,41 g/mol

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.01 (dq, J = 13.8, 6.9 Hz, 1H), 6.19 (dt, J = 15.6, 1.6 Hz, 1H), 3.59 (s, 3H), 3.27 (br s, 1H), 2.98 (t, J = 5.4 Hz, 1H), 2.23 (t, J = 7.5 Hz, 1H), 1.85 (dt, J = 7.0, 1.5 Hz, 1H), 1.66–1.47 (m, 4H), 1.45–1.33 (m, 2H), 1.33–1.13 (m, 13H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.4, 174.2, 145.5, 125.7, 58.9, 58.3, 51.4, 34.0, 31.8, 29.3, 29.23, 29.19, 29.16, 29.06, 25.8, 24.9, 18.6; **HRMS** ESI (*m/z*) calcd for $C_{17}H_{29}O_4$ [M+H$^+$]: 297.20604, found 297.20612.

Methyl 10-((2*S*,3*R*)-3-((*E*)-but-2-enoyl)oxiran-2-yl)decanoate ((+)-13). To a stirred white suspension of methylketone (+)-**11** (40.0 mg, 0.15 mmol, 1 equiv) in THF (3 mL) at –78 °C was added LiHMDS (225 µL, 1M in THF, 0.225 mmol, 1.5 equiv). After 20 min, acetaldehyde (25 µL, 0.450 mmol, 3 equiv) was added to the clear slightly yellow solution and the reaction mixture was stirred for 1 h at this temperature. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The crude

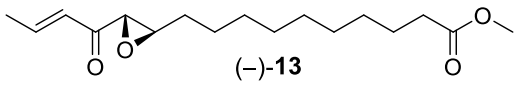
residue was filter through a plug of silica and eluted with a mixture of Hexanes/EtOAc (1:1). The residue was then purified by a plug of silica gel, eluting with 50% EtOAc/hexanes, to give the corresponding mixture of alcohols, which was taken for the next step without further characterization. Analysis of the residue by ^{1}H NMR spectroscopy *indicated the formation of a 1:1 mixture of both diastereomers*. To a solution of the residue in CH_2Cl_2 (2 mL) was subsequently added Et_3N (61 μL, 0.450 mmol, 3 equiv) and MsCl (18 μL, 0.225 mmol, 1.5 equiv) at 0 °C. The reaction was then warmed to room temperature and stirred for 1h. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The crude residue was purified by flash chromatography to afford the product (+)-**13** as a colorless oil (21.0 mg, 47% yield).



(+)-**13**
$C_{17}H_{28}O_4$
M = 296,41 g/mol

$[\alpha]_D^{20}$ +13.4 (*c* 0.67, $CHCl_3$)

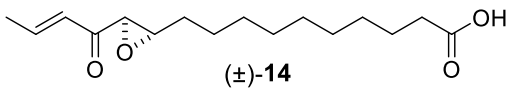
Methyl 10-((2*R*,3*S*)-3-((*E*)-but-2-enoyl)oxiran-2-yl)decanoate ((–)-13). To a stirred white suspension of methylketone (–)-**11** (40.0 mg, 0.15 mmol, 1 equiv) in THF (3 mL) at –78 °C was added LiHMDS (225 μL, 1M in THF, 0.225 mmol, 1.5 equiv). After 5 min, acetaldehyde (25 μL, 0.450 mmol, 3 equiv) was added to the clear slightly yellow solution and the reaction mixture was stirred for 1 h at this temperature. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The crude residue was filter through a plug of silica and eluted with a mixture of Hexanes/EtOAc (1:1). The residue was then purified by a plug of silica gel, eluting with 50% EtOAc/hexanes, to give the corresponding mixture of alcohols, which was taken for the next step without further characterization. Analysis of the residue by ^{1}H NMR spectroscopy *indicated the formation of a 1:1 mixture of both diastereomers*. To a solution of the residue in CH_2Cl_2 (2 mL) was subsequently added Et_3N (61 μL, 0.450 mmol, 3 equiv) and MsCl (18 μL, 0.225 mmol, 1.5 equiv) at 0 °C. The reaction was then warmed to room temperature and stirred for 1h. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The crude residue was purified by flash chromatography to afford the product (–)-**13** as a colorless oil (23.0 mg, 52% yield).



(–)-**13**
$C_{17}H_{28}O_4$
M = 296,41 g/mol

$[\alpha]_D^{20}$ –15.8 (*c* 0.45, $CHCl_3$)

10-((2*S*,3*R*)-3-((*E*)-but-2-enoyl)oxiran-2-yl)decanoic acid ((±)-14). Methyl ester (±)-**13** (21 mg, 0.071 mmol) was dissolved in a mixture of 0.4 mL of acetone and 3.6 mL phosphate buffer (pH=7). Pig liver enzyme (PLE E3019-3.5KU–Aldrich) (3 mg) was added and the cloudy white suspension was stirred at 37 ˚C for 6 hours. The final clear solution was then diluted with brine, extracted with ethyl acetate, dried over anhydrous magnesium sulfate, and concentrated *in vacuo*. The resulting oil was purified *via* column chromatography to afford (±)-**14** as a colorless oil (15 mg, 75% yield).

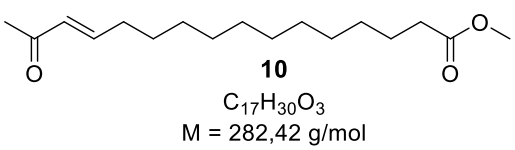


(±)-**14**
$C_{16}H_{26}O_4$
M = 282,38 g/mol

^{1}H NMR (600 MHz, $CDCl_3$) δ 10.88 (br s, 1H), (7.09 (dq, *J* = 13.8, 6.9 Hz, 1H), 6.26 (dd, *J* = 15.7, 1.6 Hz, 1H), 3.34 (d, *J* = 1.9 Hz, 1H), 3.06–3.02 (m, 1H), 2.35 (t, *J* = 7.5 Hz, 2H), 1.92 (dd, *J* = 6.9, 1.5 Hz, 3H), 1.70–1.56 (m, 5H), 1.51–1.39 (m, 3H), 1.38–1.18 (m, 18H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.7, 179.3, 145.8, 125.8, 59.1, 58.5, 34.0, 31.9, 29.8 (*grease*), 29.48, 29.37, 29.33, 29.27, 29.1, 25.9, 24.8, 18.7; **HRMS** ESI (*m/z*) calcd for $C_{16}H_{27}O_4$ $[M+H^+]$: 283.19039, found 283.19023.

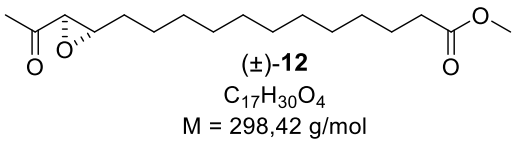
1.3. Synthesis of *post*-YM-47515 (+)-**5**

Methyl (*E*)-15-oxohexadec-13-enoate (10). In a flame dried flask equipped with a metal stir bar were added methyl tetradec-13-enoate **8** (83.0 mg, 0.345 mmol, 1 equiv) in diethyl ether (0.5M), methyl vinyl ketone (0.09 mL, 1.04 mmol, 3 equiv), Grubbs Catalyst, 2nd Generation (5.8 mg, 6.9 μmol, 2 mol %), and CuI (2.00 mg, 0.01 mmol, 3 mol %). The solution was stirred under argon at room temperature overnight, quenched with a saturated aqueous solution of ammonium chloride and extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over anhydrous magnesium sulfate, and concentrated *in vacuo*. The resulting brown residue was purified *via* column chromatography resulting in 80.0 mg of a yellow oil (83% yield).



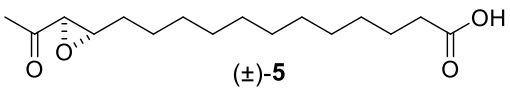
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.78 (td, J = 15.0, 6.8 Hz, 1H), 6.04 (d, J = 15.9 Hz, 1H), 3.64 (s, 3H), 2.27 (t, J = 7.0 Hz, 2H), 2.22 (s, 3H), 2.22 (m, 2H), 1.67–1.52 (m, 2H), 1.49–1.36 (m, 2H), 1.32–1.06 (m, 14H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.9, 174.4, 148.8, 131.4, 51.5, 34.2, 32.6, 29.60, 29.56, 29.49, 29.45, 29.32, 29.26, 29.22, 28.2, 26.9, 25.0; **HRMS** ESI (*m/z*) calcd for $C_{17}H_{31}O_3$ [M+H$^+$]: 283.22677, found 283.22663.

Methyl 12-((2*S,3*R**)-3-acetyloxiran-2-yl)dodecanoate ((±)-12)**. To a stirred solution of alkene **10** (104 mg, 0.36 mmol, 1 equiv) and *tert*-butylamine (2.6 mg, 0.04 mmol, 1 mol %) in methanol (2.5 mL) at 0 ˚C were slowly added 30% by weight hydrogen peroxide (0.20 mL, 1.8 mmol, 5 equiv). The solution was allowed to warm to room temperature and stirred overnight. The reaction was quenched with a 1:1 mixture of saturated aqueous sodium thiosulfate and aqueous sodium bicarbonate and extracted with three portions of dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The resulting solid was purified *via* column chromatography resulting in 48 mg of a white solid (45% yield).



^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (s, 3H), 3.15 (d, J = 1.9 Hz, 1H), 3.04 (m, 1H), 2.27 (t, J = 7.6 Hz, 2H), 2.03 (s, 3H), 1.67–1.48 (m, 2H), 1.48–1.35 (m, 4H), 1.28–1.16 (m, 14H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 206.0, 174.3, 59.9, 58.0, 51.4, 34.0, 31.7, 29.7, 29.44, 29.38, 29.37, 29.34, 29.2, 29.1, 25.7, 24.9, 24.3; **HRMS** ESI (*m/z*) calcd for $C_{17}H_{31}O_3$ [M+H$^+$]: 299.22169, found 299.22170.

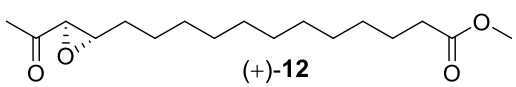
12-((2*S,3*R**)-3-acetyloxiran-2-yl)dodecanoic acid ((±)-5)**. Methyl ester **10** (24 mg, 0.08 mmol, 1 equiv) was dissolved in a mixture of 0.2 mL of acetone and 1.8 mL phosphate buffer (pH=7). Pig liver enzyme (PLE E3019-3.5KU–Aldrich) (10 mg) was added and the cloudy white suspension was stirred at 37 ˚C for 3 hours. The suspension was diluted with brine, extracted with three portions of ethyl acetate, dried over anhydrous magnesium sulfate, and concentrated *in vacuo*. The resulting white solid was purified *via* column chromatography (9 mg, 40% yield).



(±)-**5**
$C_{16}H_{28}O_4$
M = 284,40 g/mol

^{1}H NMR (600 MHz, $CDCl_3$) δ 3.18 (d, J = 1.8 Hz, 1H), 3.10-3.03 (m, 1H), 2.34 (t, J = 7.5 Hz, 2H), 2.06 (s, 3H), 1.73–1.37 (m, 6H), 1.37–1.19 (m, 14H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 206.4, 179.7, 60.1, 58.3, 34.1, 31.9, 29.8, 29.6, 29.54, 29.49, 29.4, 29.3, 29.2, 25.1, 24.8, 24.5; **HRMS** ESI (*m/z*) calcd for $C_{16}H_{29}O_4$ [M+H$^+$]: 285.20604, found 285.20586.

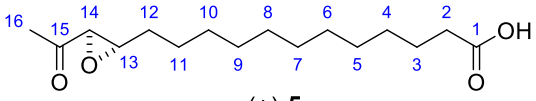
Methyl 12-((2*S*,3*R*)-3-acetyloxiran-2-yl)dodecanoate ((+)-12). 9-amino-*epi*-Quinidine (35 mg, 0.12 mmol, 30 mol %) was added to a solution of trifluoroacetic acid (67.8 mg, 0.6 mmol, 1.5 equiv) in 2 mL of dioxane. Alkene **10** (112 mg, 0.4 mmol, 1 equiv) was added and the solution was stirred at 50 ˚C. After 15 minutes, 30% by weight sodium hydroxide (0.1 mL, 0.6 mmol, 1.5 equiv) were added and the solution was stirred overnight. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with three portions of ethyl acetate. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. To the resulting white solid were added 2 mL anhydrous methanol and 1 M solution of sodium methoxide in methanol (0.4 mL, 0.4 mmol, 1 equiv). After two hours, the reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with three portions of ethyl acetate. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. Purification was performed by column chromatography resulting in 40.3 mg of a low melting point off-white solid (40 mg, 34% yield).



(+)-**12**
$C_{17}H_{30}O_4$
M = 298,42 g/mol

$[\alpha]_D^{20}$ +14.5 (*c* 1.00, $CHCl_3$)

12-((2*S*,3*R*)-3-acetyloxiran-2-yl)dodecanoic acid ((+)-5). Methyl ester (+)-**12** (20 mg, 0.07 mmol, 1 equiv) was dissolved in a mixture of 0.2 mL of acetone and 1.8 mL phosphate buffer (pH=7). Pig liver enzyme (PLE E3019-3.5KU–Aldrich) (10 mg) were added and the cloudy white suspension was stirred at 37 ˚C for 3 hours. The suspension was diluted with brine, extracted with ethyl acetate, dried over anhydrous magnesium sulfate, and concentrated *in vacuo*. The resulting low melting point white solid was purified *via* column chromatography (16 mg, 80% yield).



(+)-**5**

$C_{16}H_{28}O_4$

M = 284,40 g/mol

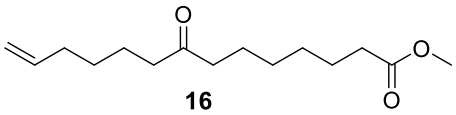
^{1}H NMR (600 MHz, CD_3OD) δ 3.24 (d, J = 1.9 Hz, 1H), 3.12 (ddd, J = 6.4, 3.6, 1.8 Hz, 2H), 2.27 (t, J = 7.4 Hz, 2H), 2.06 (s, 3H), 1.51–1.75 (m, 6H), 1.42-1.52 (m, 2H), 1.16-1.43 (m, 12H); **^{13}C NMR** (150 MHz, CD_3OD) δ 208.0 177.9, 60.8, 59.4, 35.1, 32.9, 30.63, 30.60, 30.57, 30.56, 30.41, 30.38, 30.24, 26.9, 26.1, 24.8; **$[\alpha]_D^{20}$** +3.3 (*c* 0.28, MeOH)

Supplementary Table S3. Comparison of ^{1}H and ^{13}C NMR spectra of (+)-**5** and the natural product (CD_3OD).

	δ_H			δ_C	
	Natural (500 MHz)	**Synthetic (600 MHz)**		**Natural (500 MHz)**	**Synthetic (600 MHz)**
1	-[a]	-		179.0	177.9
2	2.24, t (7.7)	2.27, t (7.4)		36.0	35.1
3	1.59, m	1.60, m		26.5	26.1
4	1.30, m	1.43, m		30.5	30.56
5	1.28-1.67	1.16-1.43		26.9-30.8	26.9-30.63
6					
7					
8					
9					
10					
11					
12	1.57, m	1.60, m		32.9	32.9
13	3.11, td (5.5, 1.8)	3.12, ddd (6.4, 3.6, 1.8)		59.5	59.4
14	3.23 d (1.8)	3.24, d (1.8)		60.9	60.8
15	-[a]	-		208.0	208.0
16	2.06, s	2.06, s		24.8	24.8

1.4. Synthesis of *post*-amycomicin (–)-**6**

Methyl 8-oxotetradec-13-enoate (16). A solution of anhydrous zinc chloride (136 mg, 1.00 mmol, 1 equiv) in anhydrous Et_2O (10 mL) was treated with freshly prepared hex-5-enylmagnesium bromide (0.9 equiv) dropwise at –78 °C. The temperature was increased to 0 °C and the reaction mixture was treated with acyl chloride (207 mg, 1.00 mmol, 1 equiv) in anhydrous THF (10 mL) followed by $Pd(PPh_3)_4$ (57.8 mg, 0.0500 mmol, 5 mol %). The resulting mixture was stirred at 0 °C for 30 minutes, then at room temperature for 1.5 h. The reaction was quenched by the addition of 1N HCl (2 mL) and extracted twice with Et_2O. The combined organic layers were washed with saturated aqueous solution of $NaHCO_3$, dried with $MgSO_4$ and concentrated. The residue was purified by flash chromatography to afford the product **16** as a colorless oil (216 mg, 85% yield).



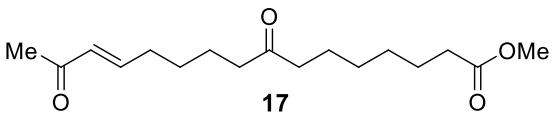
16

$C_{15}H_{26}O_3$

M = 254,37 g/mol

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.79 (ddt, J = 17.0, 10.2, 6.7 Hz, 1H), 5.00 (ddd, J = 17.0, 3.4, 1.6 Hz, 1H), 4.95 (dd, J = 10.2, 0.9 Hz, 1H), 3.66 (s, 3H), 2.39 (td, J = 7.4, 5.2 Hz, 2H), 2.30 (td, J = 7.5, 2.8 Hz, 2H), 2.05 (app q, J = 7.2 Hz, 2H), 1.66–1.54 (m, 8H), 1.42–1.24 (m, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 211.4, 174.4, 138.7, 114.8, 51.6, 42.82, 42.77, 34.1, 33.7, 29.06, 29.01, 28.6, 24.9, 23.8, 23.5; **HRMS** ESI (*m/z*) calcd for $C_{15}H_{26}O_3Na$ [M+Na$^+$]: 277.17742, found 277.17751.

Methyl (*E*)-8,15-dioxohexadec-13-enoate (17). In a flame dried flask equipped with a metal stir bar were added alkene **16** (110 mg, 0.432 mmol, 1 equiv) in diethyl ether (0.5M), methyl vinyl ketone (108 µL, 1.30 mmol, 3 equiv), Grubbs Catalyst, 2nd Generation (7.6 mg, 0.009 mmol, 2 mol %), and CuI (2.5 mg, 0.013 mmol, 3 mol %). The solution was stirred under argon at room temperature overnight, quenched with a saturated aqueous solution of ammonium chloride and extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over anhydrous magnesium sulfate, and concentrated *in vacuo*. The resulting brown residue was purified *via* column chromatography resulting in 83.0 mg of a yellow oil (65% yield).



17

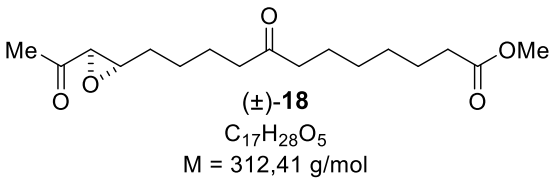
$C_{17}H_{28}O_4$

M = 296,41 g/mol

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.78 (dt, J = 15.9, 6.9 Hz, 1H), 6.07 (d, J = 16.0 Hz, 1H), 3.66 (s, 3H), 2.40 (dt, J = 16.9, 7.4 Hz, 4H), 2.30 (t, J = 7.5 Hz, 2H), 2.26–2.20 (m, 2H), 2.24 (s, 3H), 1.65–1.53 (m, 6H), 1.50–1.43 (m, 2H), 1.35–1.26 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 210.9, 198.8, 174.3, 147.9, 131.7, 51.6, 42.9, 42.5, 34.1, 32.4, 29.03, 28.99, 27.8, 27.1, 24.9, 23.7, 23.4; **HRMS** ESI (*m/z*) calcd for $C_{17}H_{28}O_4Na$ [M+Na$^+$]: 319.18798, found 319.18785.

Methyl 12-((2*S,3*R**)-3-acetyloxiran-2-yl)-8-oxododecanoate ((±)-18).** To a stirred solution of alkene **16** (83 mg, 0.28 mmol, 1 equiv) and *tert*-butylamine (1.8 mg, 0.03 mmol, 1 mol %) in methanol (2.2 mL) at 0 ˚C were slowly added 30% by weight hydrogen peroxide (160 µL, 1.12 mmol, 5 equiv). The solution was allowed to warm to room temperature and stirred overnight. The reaction was quenched with a 1:1 mixture of saturated sodium thiosulfate and sodium bicarbonate and extracted with three portions of dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The

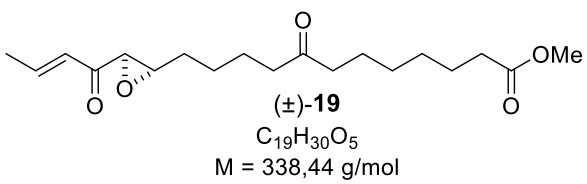
resulting oil was purified *via* column chromatography to afford epoxide (±)-**18** as a colorless oil (63 mg, 69% yield).



(±)-**18**
$C_{17}H_{28}O_5$
M = 312,41 g/mol

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64 (s, 3H), 3.16 (d, J = 2.0 Hz, 1H), 3.06 (ddd, J = 6.5, 4.7, 2.0 Hz, 1H), 2.38 (dt, J = 11.7, 7.3 Hz, 4H), 2.28 (t, J = 7.5 Hz, 2H), 2.04 (s, 3H), 1.76–1.49 (m, 8H), 1.49–1.37 (m, 2H), 1.35–1.20 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 210.8, 206.1, 174.3, 59.9, 57.9, 51.6, 42.8, 42.4, 34.1, 31.7, 28.98, 28.93, 25.5, 24.8, 24.5, 23.7, 23.3; **HRMS** ESI (*m/z*) calcd for $C_{17}H_{29}O_5$ [M+H$^+$]: 313.20095, found 313.20108.

Methyl 12-((2*S,3*R**)-3-((*E*)-but-2-enoyl)oxiran-2-yl)-8-oxododecanoate ((±)-19).** To a stirred white suspension of methylketone (±)-**18** (40.0 mg, 0.128 mmol, 1 equiv) in THF (3 mL) at –78 °C was added LiHMDS (192 µL, 1M in THF, 0.192 mmol, 1.5 equiv). After 5 min, acetaldehyde (22 µL, 0.384 mmol, 3 equiv) was added to the clear slightly yellow solution and the reaction mixture was stirred for 1 h at this temperature. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The crude residue was filter through a plug of silica and eluted with a mixture of Hexanes/EtOAc (1:1). The residue was then purified by a plug of silica gel, eluting with 50% EtOAc/hexanes, to give the corresponding mixture of alcohols, which was taken for the next step without further characterization. Analysis of the residue by ^{1}H NMR spectroscopy *indicated the formation of a 1:1 mixture of both diastereomers*. To a solution of the residue in CH_2Cl_2 (2 mL) was subsequently added Et_3N (52 µL, 0.384 mmol, 3 equiv) and MsCl (52 µL, 0.384 mmol, 3 equiv) at 0 °C. The reaction was then warmed to room temperature and stirred for 1h. The reaction was quenched with a saturated aqueous solution of ammonium chloride and extracted with EtOAc. The combined organic layers were dried over anhydrous magnesium sulfate and concentrated *in vacuo*. The crude residue was purified by flash chromatography to afford the product (±)-**19** as a colorless oil (24.0 mg, 55% yield).

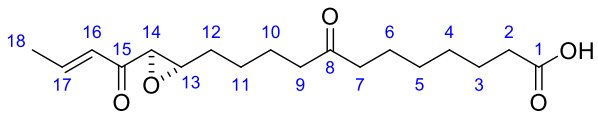


(±)-**19**
$C_{19}H_{30}O_5$
M = 338,44 g/mol

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (dq, J = 13.9, 6.9 Hz, 1H), 6.26 (dd, J = 15.7, 1.5 Hz, 1H), 3.66 (s, 3H), 3.34 (d, J = 1.8 Hz, 1H), 3.06–3.03 (m, 1H), 2.45–2.35 (m, 4H), 2.30 (t, J = 7.5 Hz, 2H), 1.92 (dd, J = 6.9, 1.5 Hz, 3H), 1.74–1.53 (m, 8H), 1.50–1.41 (m, 2H), 1.35–

1.22 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 210.9, 195.5, 174.3, 145.9, 125.8, 59.0, 58.1, 51.6, 42.9, 42.5, 34.1, 31.8, 29.03, 28.99, 25.6, 24.9, 23.7, 23.4, 18.7; **HRMS** ESI (*m/z*) calcd for $C_{19}H_{31}O_5$ [M+H$^+$]: 339.21660, found 339.21677.

12-((2*S,3*R**)-3-((*E*)-But-2-enoyl)oxiran-2-yl)-8-oxododecanoic acid ((±)-6).** Methyl ester (±)-**19** (10 mg, 0.03 mmol, 1 equiv) was dissolved in a mixture of 0.2 mL of acetone and 1.8 mL phosphate buffer (pH=7). Pig liver enzyme (PLE E3019-3.5KU–Aldrich) (2 mg) was added and the cloudy white suspension was stirred at 37 ˚C for 5 hours. The final clear solution was then diluted with brine, extracted with ethyl acetate, dried over anhydrous magnesium sulfate, and concentrated *in vacuo*. The resulting oil was purified *via* column chromatography to afford (±)-**6** as a colorless oil (4.3 mg, 45% yield).



(±)-**6**
$C_{18}H_{28}O_5$
M = 324,42 g/mol

^{1}H NMR (600 MHz, CD_3OD) δ 7.15 (dq, J = 13.9, 6.9 Hz, 1H), 6.33 (d, J = 15.8 Hz, 1H), 3.54 (s, 1H), 3.05 (t, J = 5.3 Hz, 1H), 2.51 (t, J = 7.4 Hz, 2H), 2.48 (t, J = 7.5 Hz, 2H), 2.30 (t, J = 7.4 Hz, 2H), 1.96 (d, J = 6.9 Hz, 3H), 1.75–1.68 (m, 1H), 1.68–1.60 (m, 5H), 1.60–1.54 (m, 2H), 1.53–1.44 (m, 2H), 1.41–1.29 (m, 4H); **^{13}C NMR** (150 MHz, CD_3OD) δ 213.7, 197.2, 177.8, 147.3, 128.0, 59.7, 59.3, 43.4, 43.1, 35.1, 32.6, 29.99, 29.93, 26.4, 26.0, 24.7, 24.4, 18.7; **HRMS** ESI (*m/z*) calcd for $C_{18}H_{28}O_5Na$ [M+Na$^+$]: 347.18290, found 347.18231.

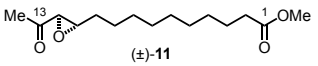
Supplementary Table S2. Comparison of ^{1}H and ^{13}C NMR spectra of **6** and the natural product (CD_3OD).

	δ_H			δ_C	
	Natural (600 MHz)	**Synthetic (600 MHz)**		**Natural (600 MHz)**	**Synthetic (600 MHz)**
1	-	-		177.0	177.9
2	2.27, t (7.4)	2.30, t (7.4)		34.8	35.1
3	1.60, m	1.68–1.60, m		25.6	26.0
4	1.34, m	1.41–1.29, m		29.5	29.9
5	1.31, m	1.41–1.29, m		29.9	30.0
6	1.56, m	1.60–1.54, m		24.4	24.7
7	2.45, t (7.4)	2.48, t (7.5)		43.1	43.4
8	-	-		212.9	213.7
9	2.49, t (7.2)	2.51, t (7.4)		42.8	43.1
10	1.61, m	1.68–1.60, m		24.1	24.4
11	1.46, m	1.53–1.44, m		26.1	26.4
12	1.62, m 1.69, m	1.75–1.68, m 1.68–1.60, m		32.3	32.6
13	3.03, ddd (11.1, 4.9, 2.0)	3.05, app t (5.3)		59.2	59.7

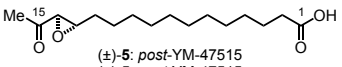
14	3.51, d (2.0)	3.54, s		58.6	59.3
15	-	-		196.9	197.2
16	6.30, dq (15.8, 1.7)	6.33, d (15.8)		127.6	128.0
17	7.14, dq (15.8, 6.9)	7.15, dq (13.9, 6.9)		147.1	147.3
18	1.94, dd (6.9, 1.7)	1.96, d (6.9)		18.4	18.7

2. Biology

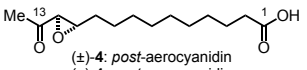
2.1. **Table S1.** Biological Evaluation



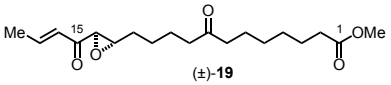
(±)-**11**



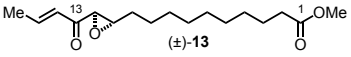
(±)-**5**: *post*-YM-47515
(+)-**5**: *post*-YM-47515



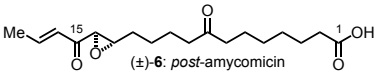
(±)-**4**: *post*-aerocyanidin
(+)-**4**: *post*-aerocyanidin



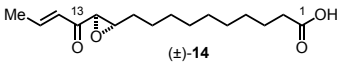
(±)-**19**



(±)-**13**



(±)-**6**: *post*-amycomicin



(±)-**14**

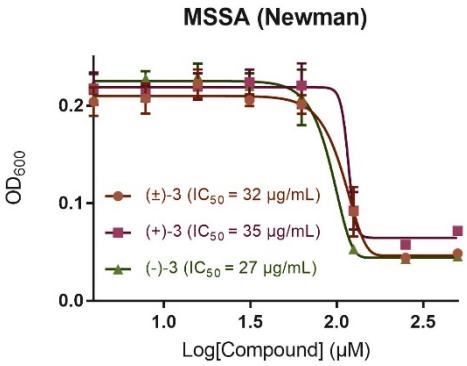
	MIC[a,b] (μM)						
	S. aureus (CA-MRSA)	*S. aureus* (HA-MRSA)	*S. aureus* (MSSA)	*E. faecalis*	*B. subtilis*	*E. coli*	*P. aeruginosa*
compound	(USA300)	(ATCC 33592)	(Newman)	(ATCC 51575)	(ATCC 6633)	(MC4100)	(PAO1)
(±)-**11**	>500	-	-	-	-	-	-
(±)-**4**: *post*-aerocyanidin	>500	-	-	-	-	-	-
(+)-**4**: *post*-aerocyanidin	>500	-	-	-	-	-	-
(±)-**13**	**250**	**250**	**250**	**250**	>500	>500	**250**
(−)-**13**	**125**	**250**	**125**	**250**	-	-	**250**
(+)-**13**	**250**	**250**	**250**	**250**	-	-	**250**
(±)-**14**	>500	-	-	-	-	-	-
(±)-**5**: *post*-YM-47515	>500	-	-	-	-	-	-
(−)-**5**: *post*-YM-47515	>500	-	-	-	-	-	-
(±)-**19**	>500	-	-	-	-	-	-
(±)-**6**: *post*-amycomicin	>500	-	-	-	-	-	-

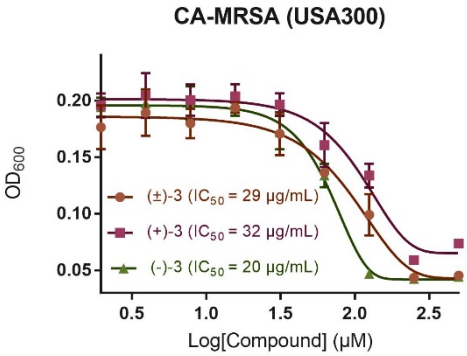
[a] Quaternary ammonium cation (12,3,2,3,12) was used as a positive control, [b] These assays were realized in triplicate and over 16 h.

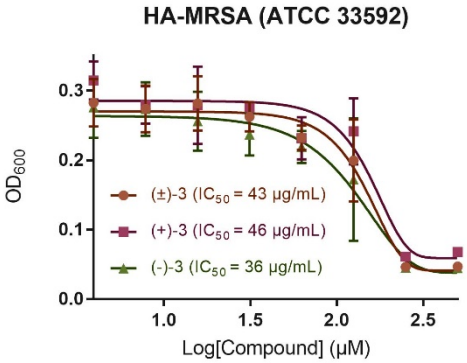
2.2. IC_{50} Assay Procedures

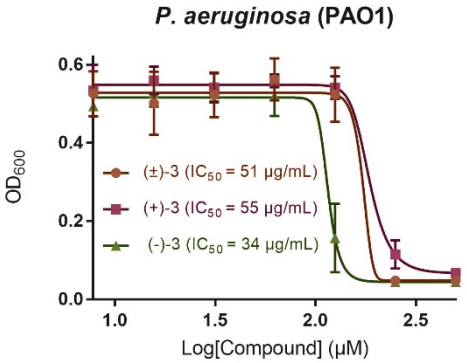
Overnight cultures of the indicated bacteria were diluted 1:100 in fresh LB media, and regrown at 37 °C with 200 rpm shaking. When the cultures reached mid-log phase, bacteria were diluted to a concentration of 0.004 using the following equation: (x μL O/N)(OD reading) = (0.004)(volume needed) and 100 μL was inoculated into each well of a 96-well plate (Corning ® 96-well clear bottom plates), which contained 100 μL of serially diluted compound. Compound serial dilutions were done starting from a 10 mM stock solution in DMSO, which was diluted with LB media to arrive at the desired final concentration. 96-well plates were grown statically at 37 °C for 16 hours, upon which time the OD at 595 nm was measured using a plate reader. IC_{50} values were calculated by fitting the OD readings in triplicate from separate O/N cultures vs. concentration with a 5-parameter-logistic model. The MIC value reflects the lowest concentration where no growth was visualized, and each assay was performed in triplicate

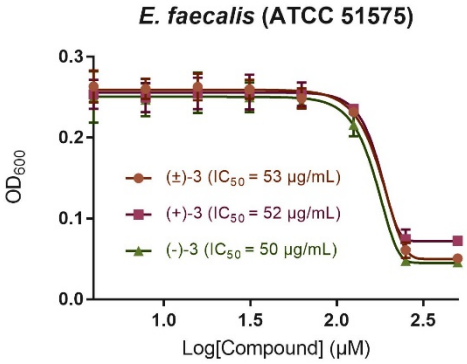
2.3. IC_{50} Assay Curves



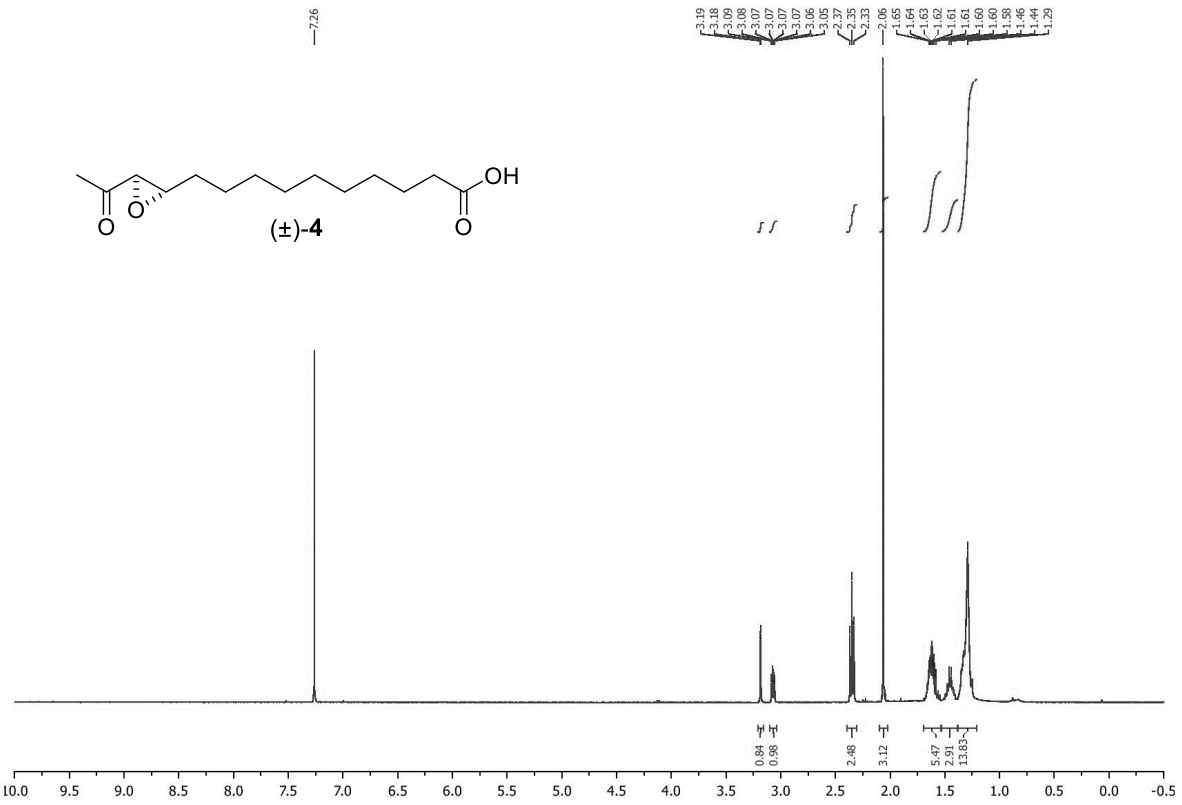


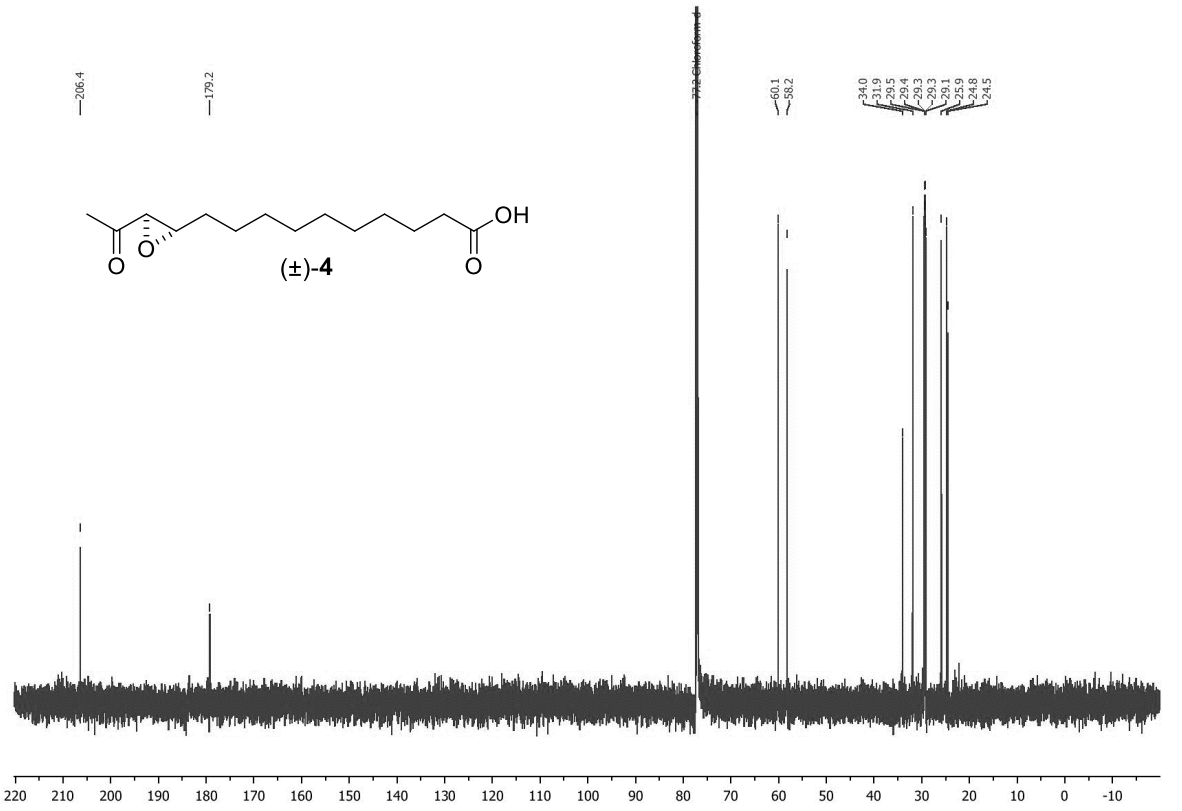


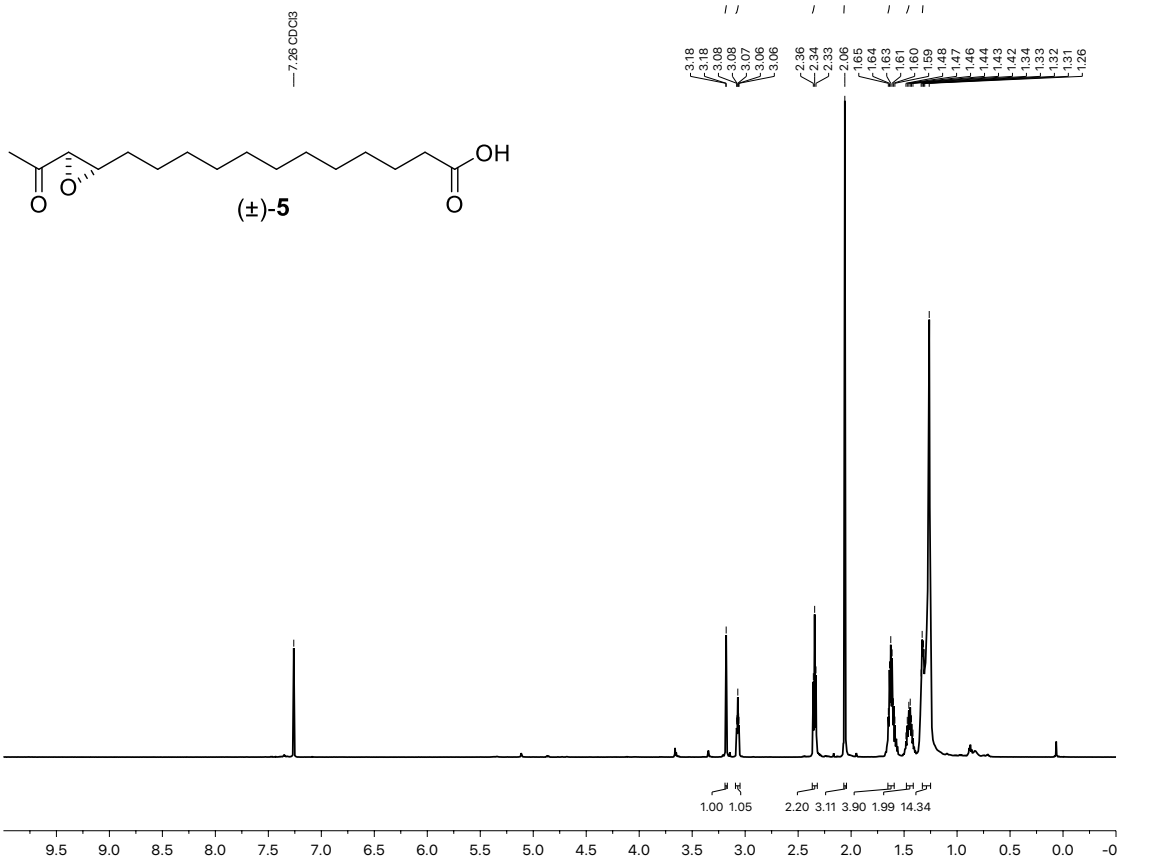




3. Appendix: Spectral Data



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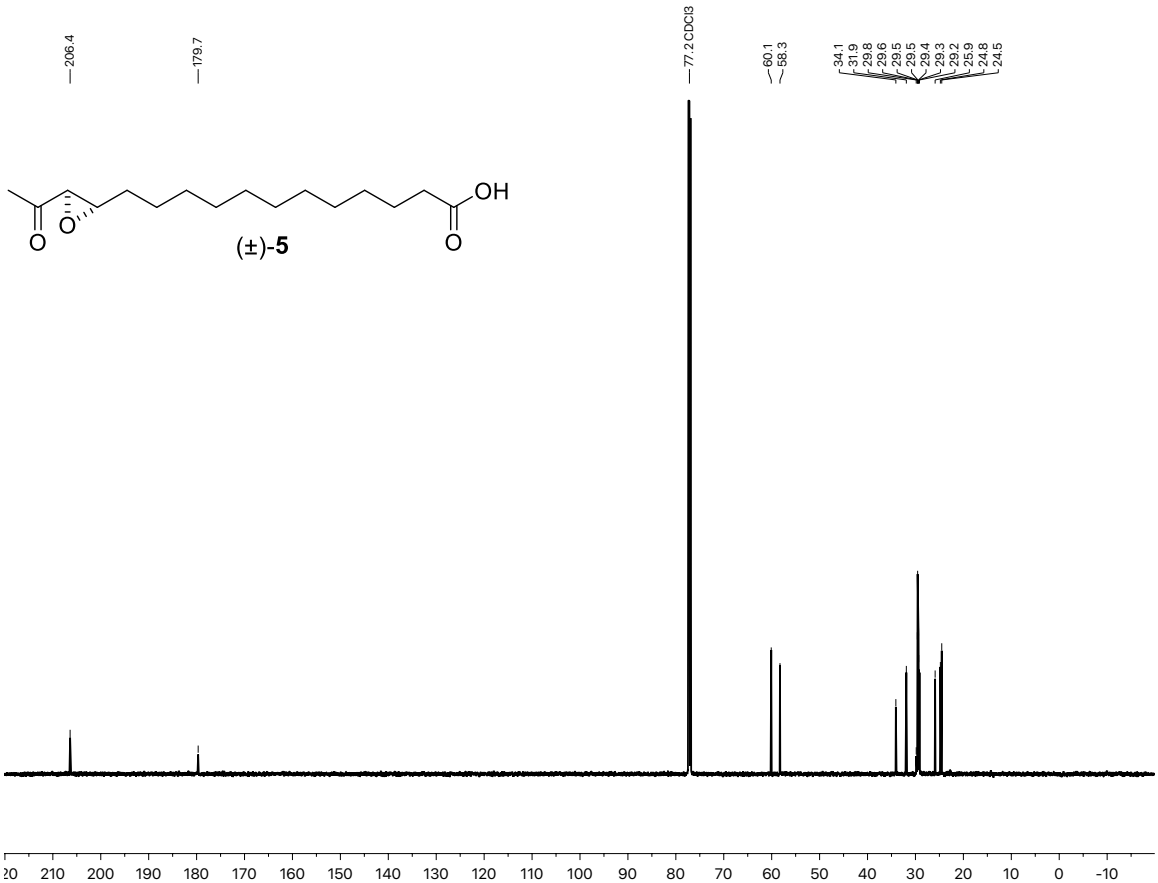
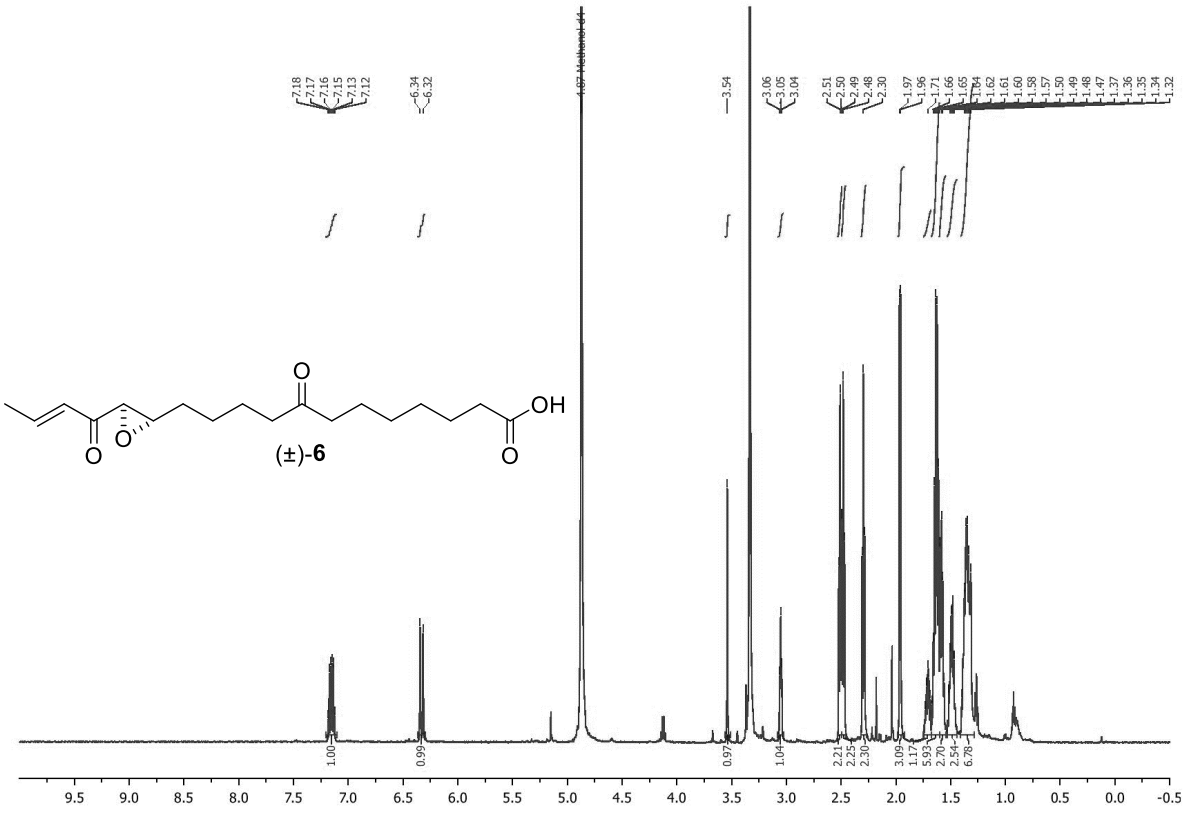
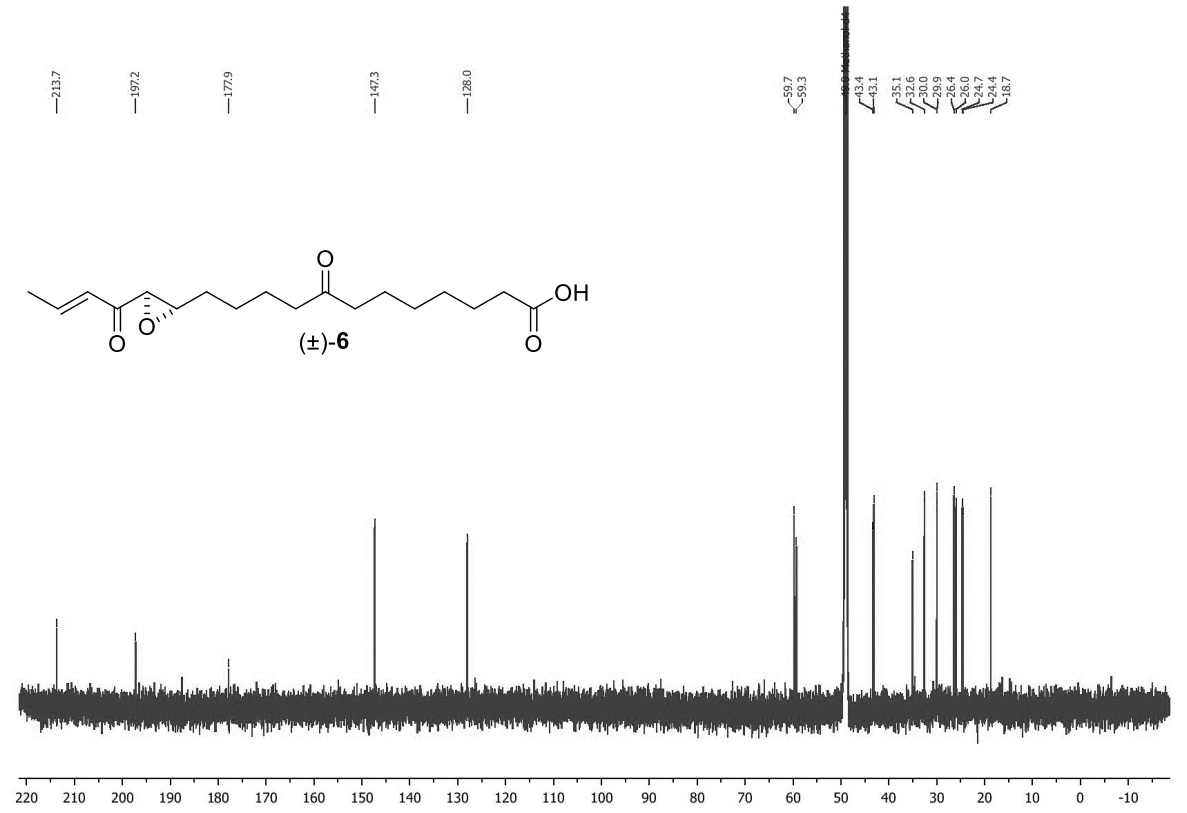
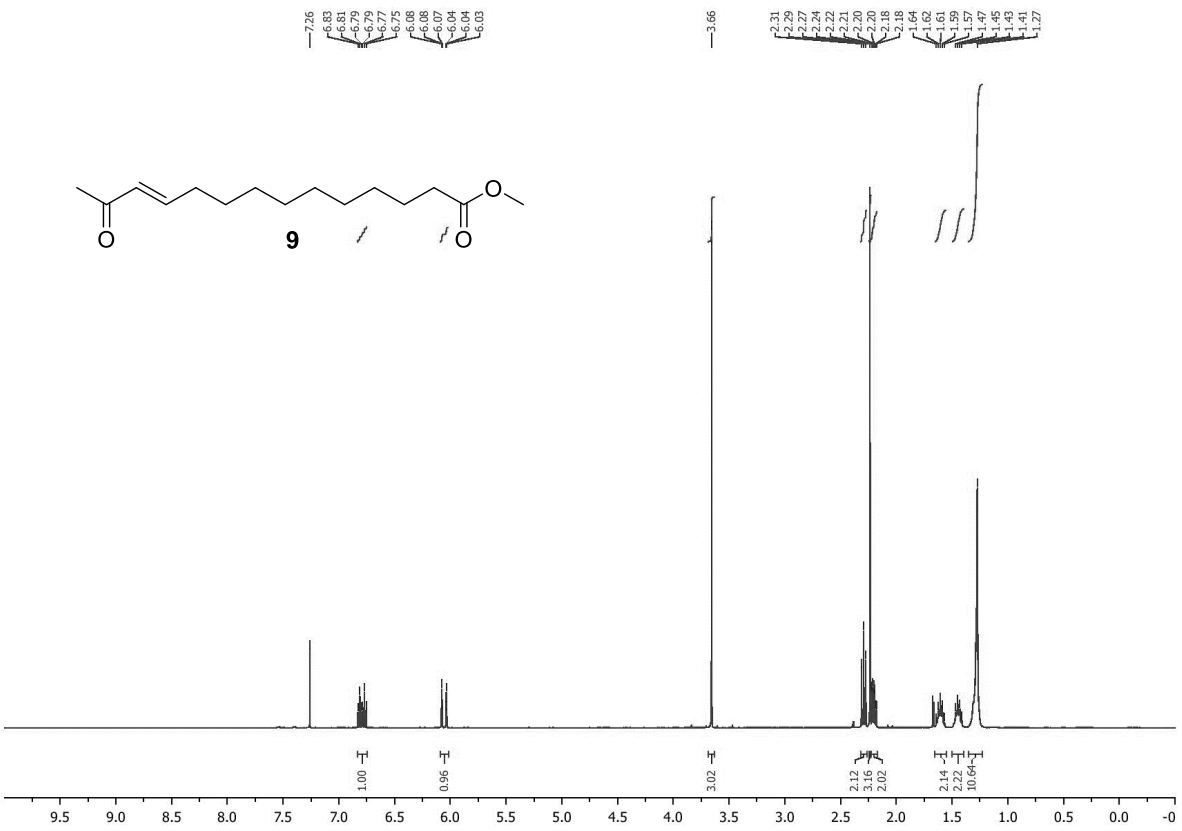
3.18
3.08
3.08
3.07
3.06
3.06
2.36
2.34
2.33
2.06
1.65
1.64
1.63
1.61
1.60
1.59
1.48
1.47
1.46
1.44
1.43
1.42
1.34
1.33
1.32
1.31
1.26
OH
O
O
(±)-5
1.00 1.05
2.20 3.11 3.90 1.99 14.34
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0


206.4
179.7
77.2 CDCl3
60.1
58.3
34.1
31.9
29.8
29.6
29.5
29.5
29.4
29.3
29.2
25.9
24.8
24.5
OH
O
O
(±)-5
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


(±)-6


(±)-6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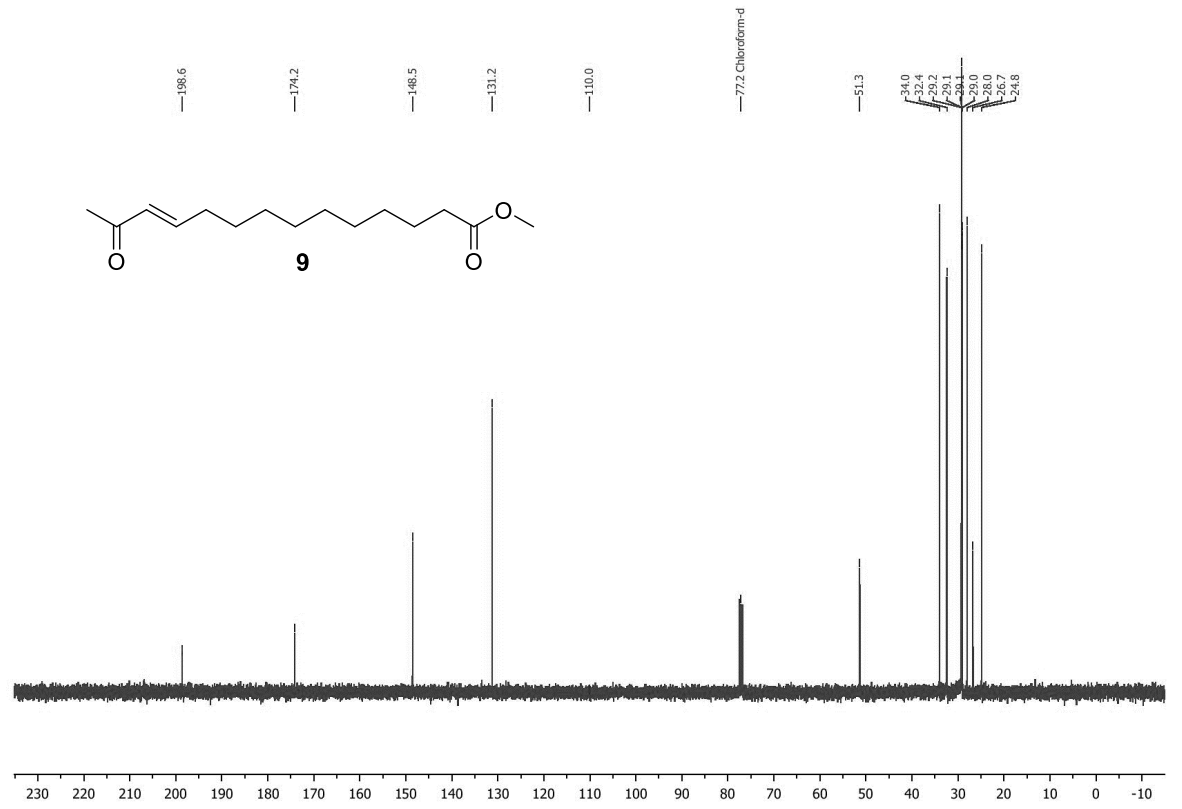
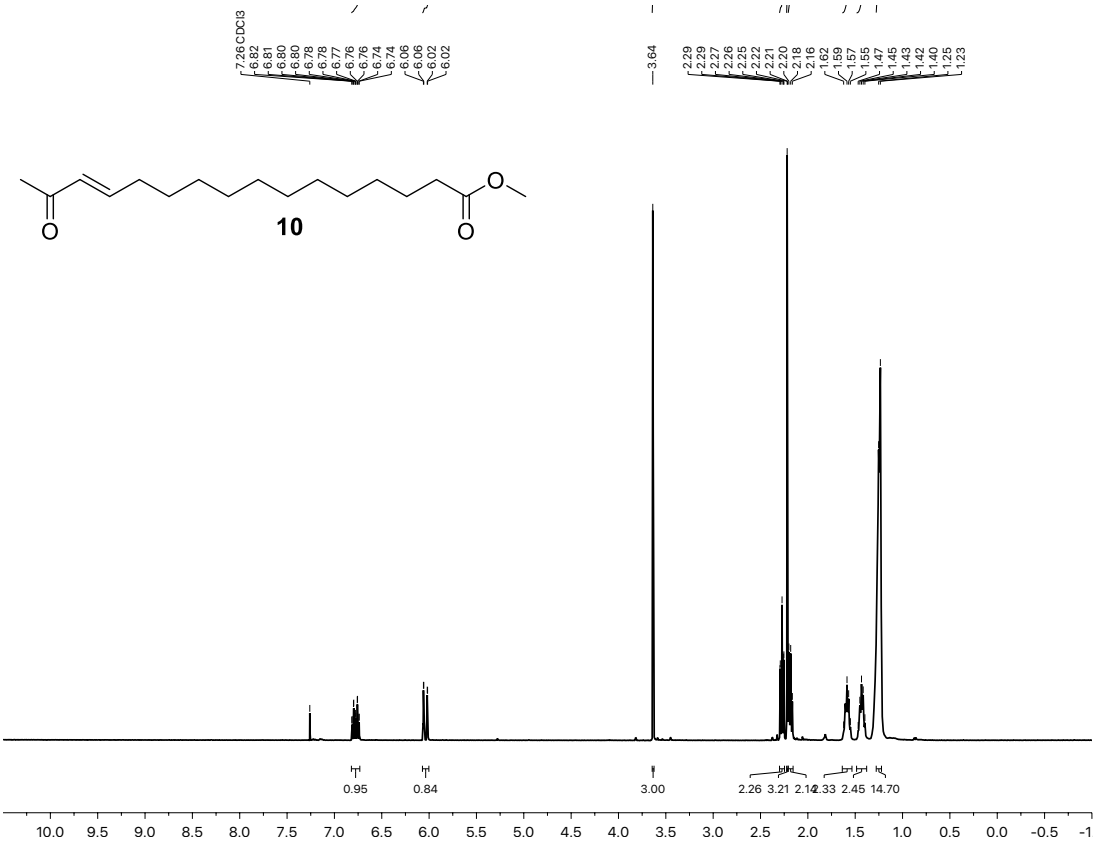
6.83
6.81
6.79
6.79
6.77
6.75
6.08
6.08
6.07
6.04
6.04
6.03
3.66
2.31
2.29
2.27
2.24
2.22
2.21
2.20
2.20
2.18
2.18
1.64
1.62
1.61
1.59
1.57
1.47
1.45
1.43
1.41
1.27
O
O
9
O
1.00
0.96
3.02
2.12
3.16
2.02
2.14
2.22
10.64
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0


198.6
174.2
148.5
131.2
110.0
77.2 Chloroform-d
51.3
34.0
32.4
29.2
29.1
29.1
29.0
28.0
26.7
24.8
O
O
9
O
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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6.80
6.80
6.78
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6.77
6.76
6.76
6.74
6.74
6.06
6.06
6.02
6.02
3.64
2.29
2.29
2.27
2.26
2.25
2.22
2.21
2.20
2.18
2.16
1.62
1.59
1.57
1.55
1.47
1.45
1.43
1.42
1.40
1.25
1.23
O
O
O
10
0.95
0.84
3.00
2.26
3.21
2.14
2.33
2.45
14.70
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
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1.0
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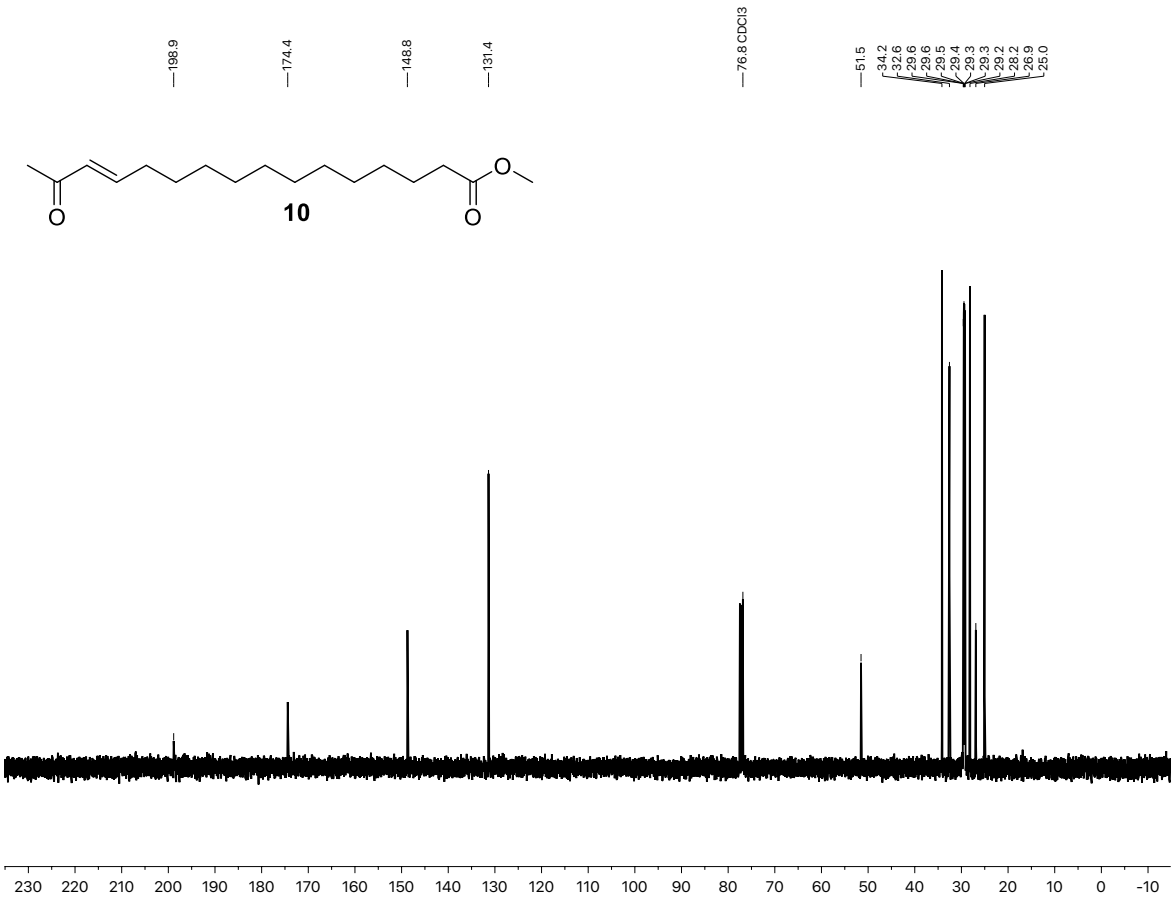
-0.5
-1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131.4
76.8 CDCl3
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34.2
32.6
29.6
29.6
29.5
29.4
29.3
29.3
29.2
28.2
26.9
25.0
O
O
O
10
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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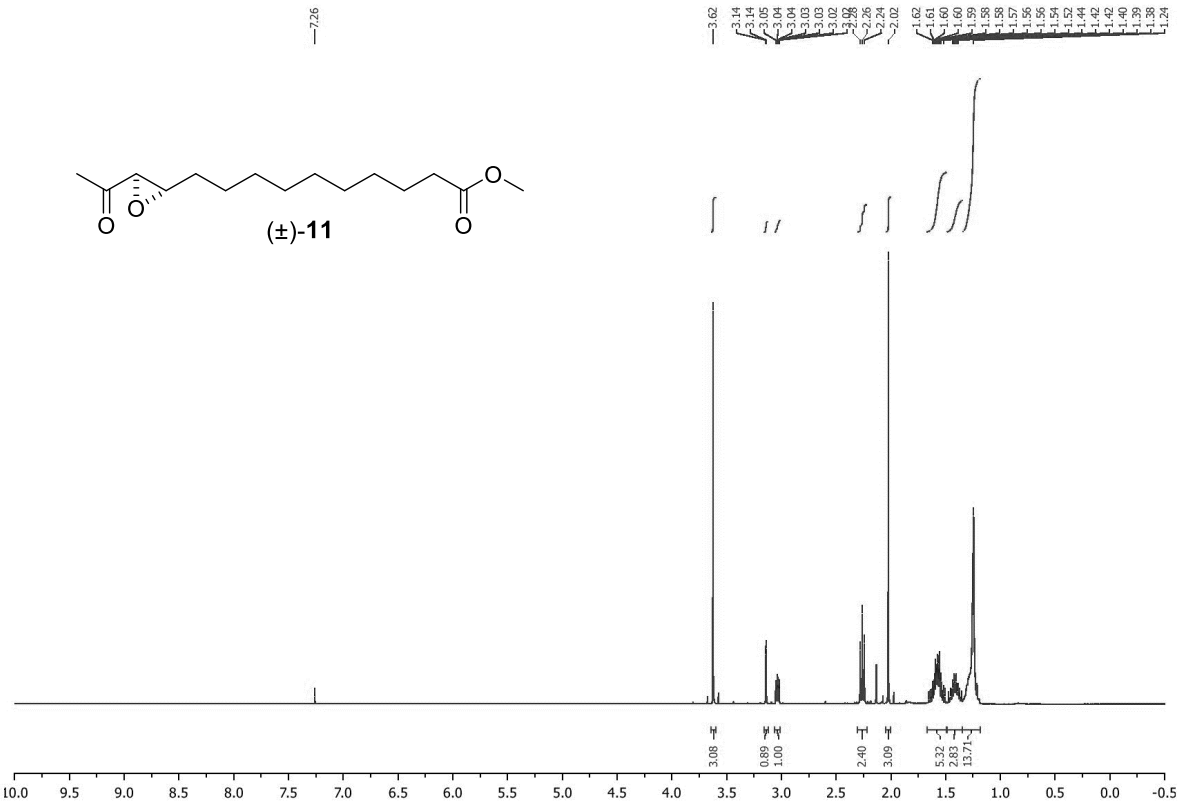
30
20
10
0
-10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3.14
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3.04
3.04
3.03
3.03
3.02
2.98
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2.02
1.62
1.61
1.60
1.60
1.59
1.58
1.58
1.57
1.56
1.55
1.54
1.52
1.44
1.42
1.42
1.40
1.39
1.38
1.24
O
O
O
O
(±)-11
3.08
0.89
1.00
2.40
3.09
5.32
2.83
13.71
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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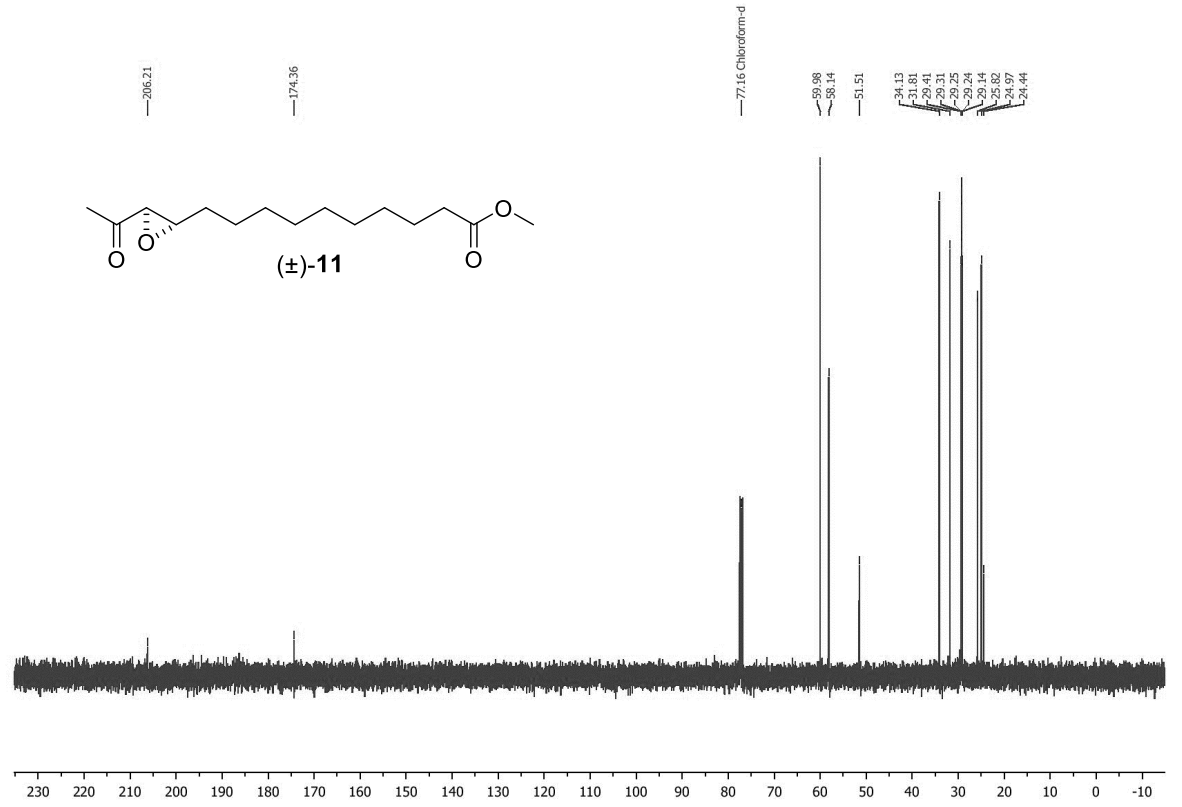
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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174.36
77.16 Chloroform-d
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58.14
51.51
34.13
31.81
29.41
29.31
29.25
29.24
29.14
25.82
24.97
24.44
O
O
O
O
(±)-11
230
220
210
200
190
180
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140
130
120
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100
90
80
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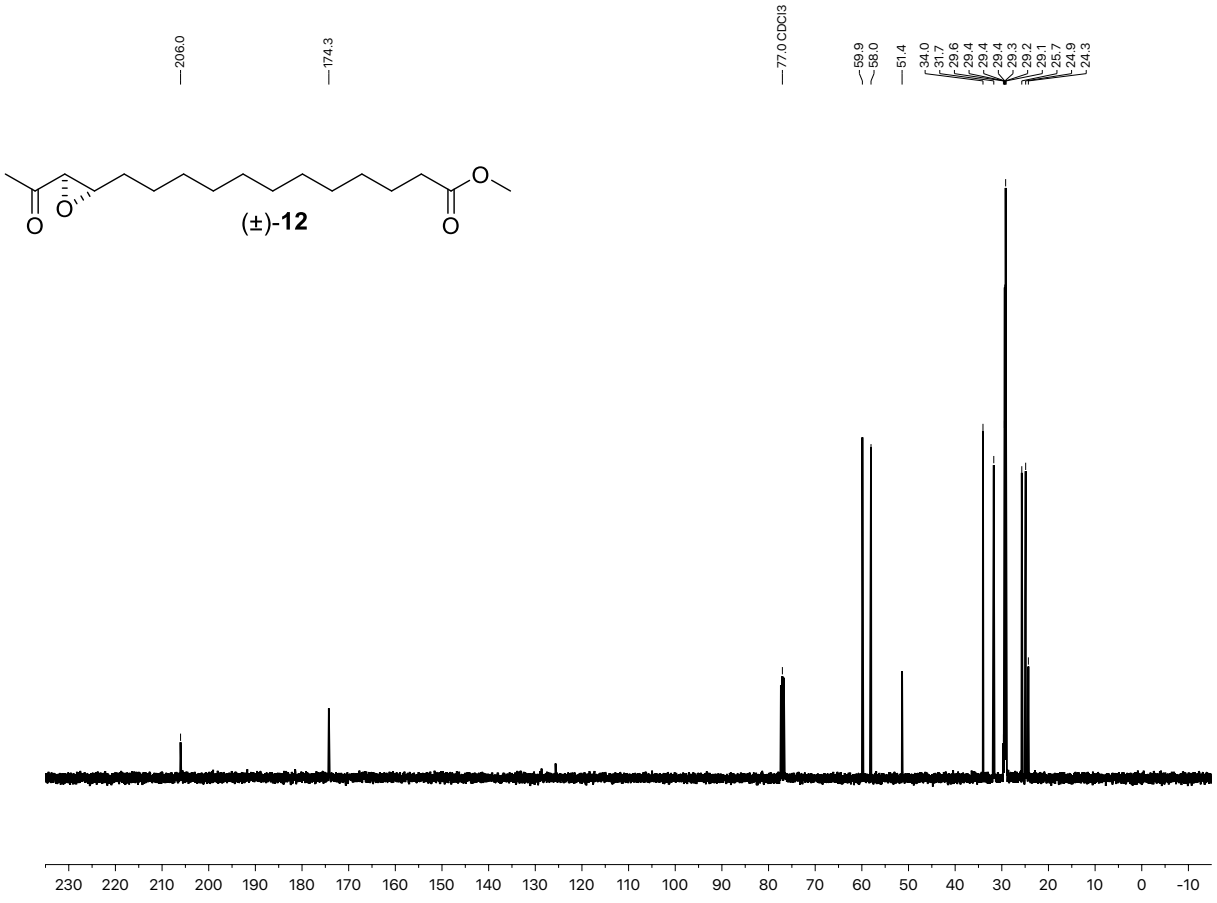
60
50
40
30
20
10
0
-10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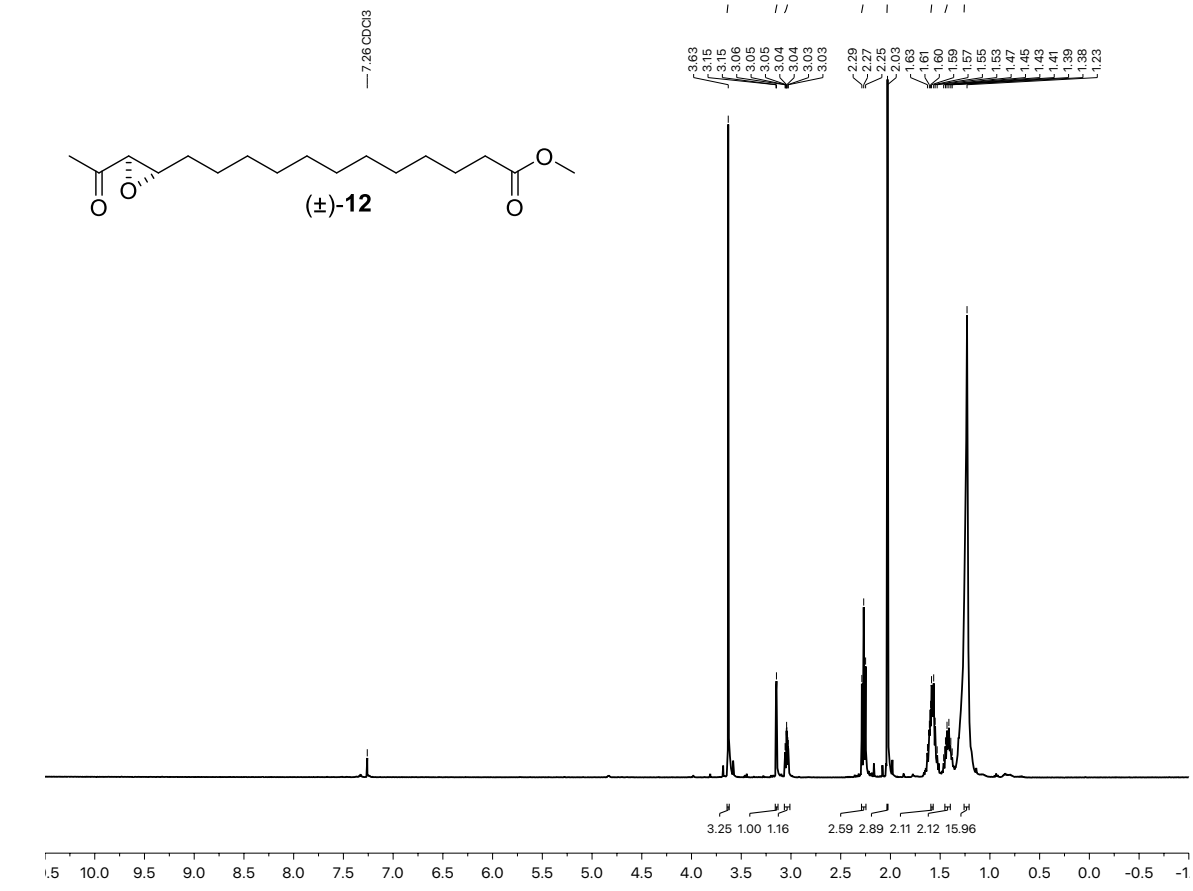
174.3
77.0 CDCl3
59.9
58.0
51.4
34.0
31.7
29.6
29.4
29.4
29.4
29.3
29.2
29.1
25.7
24.9
24.3
(±)-12
O
O
O
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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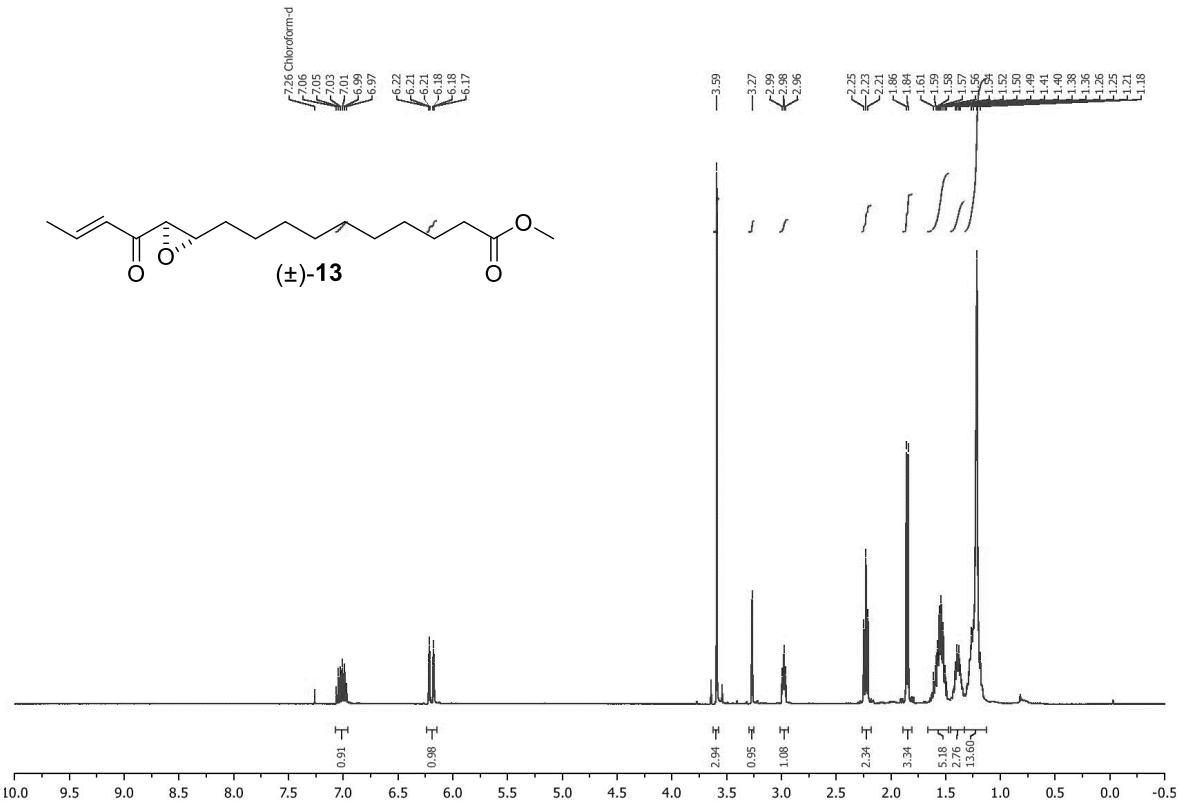
3.05
3.04
3.04
3.03
3.03
2.29
2.27
2.25
2.03
1.63
1.61
1.60
1.59
1.57
1.55
1.53
1.47
1.45
1.43
1.41
1.39
1.38
1.23
(±)-12
O
O
O
O
3.25 1.00 1.16
2.59 2.89 2.11 2.12 15.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


7.26 Chloroform-d
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7.05
7.03
7.01
6.99
6.97
6.22
6.21
6.21
6.18
6.18
6.17
3.59
3.27
2.99
2.98
2.96
2.25
2.23
2.21
1.86
1.84
1.61
1.59
1.58
1.57
1.56
1.54
1.52
1.50
1.49
1.41
1.40
1.38
1.36
1.26
1.25
1.21
1.18
(±)-13
0.91
0.98
2.94
0.95
1.08
2.34
3.34
5.18
2.76
13.60
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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1.5
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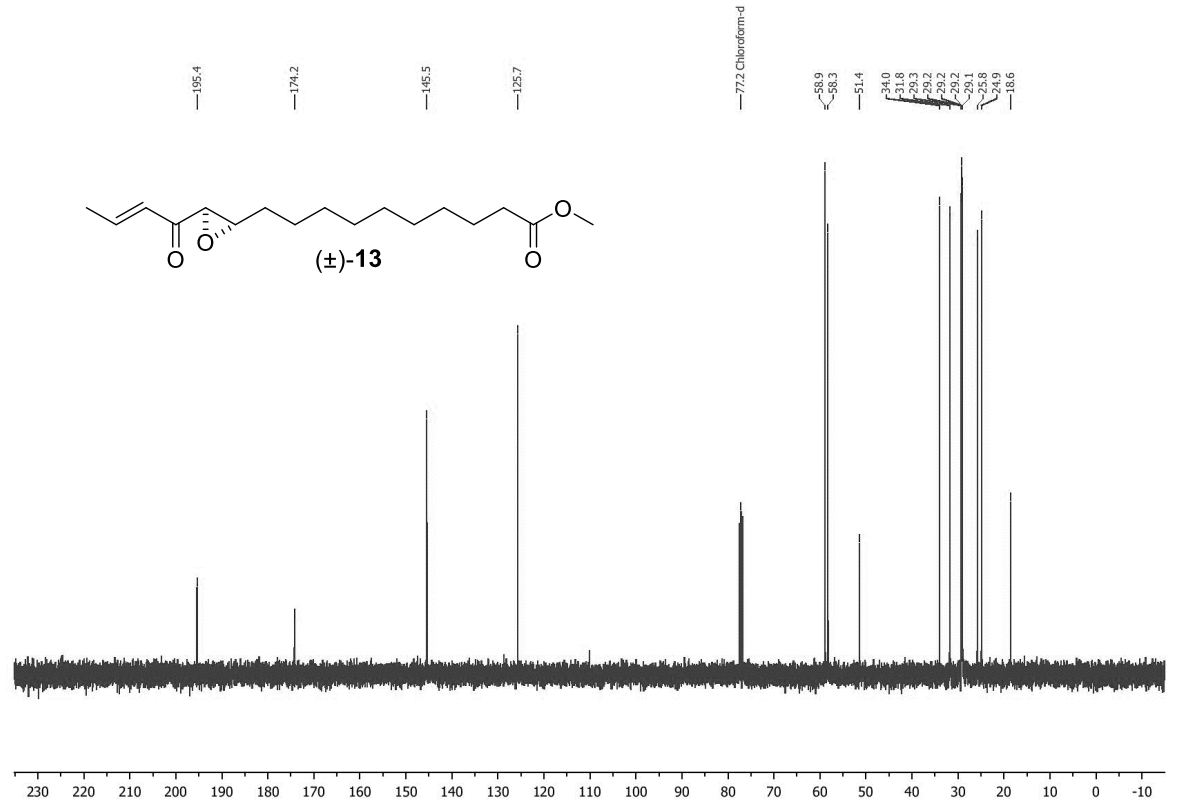
0.5
0.0
-0.5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174.2
145.5
125.7
77.2 Chloroform-d
58.9
58.3
51.4
34.0
31.8
29.3
29.2
29.2
29.2
29.1
25.8
24.9
18.6
(±)-13
230
220
210
200
190
180
170
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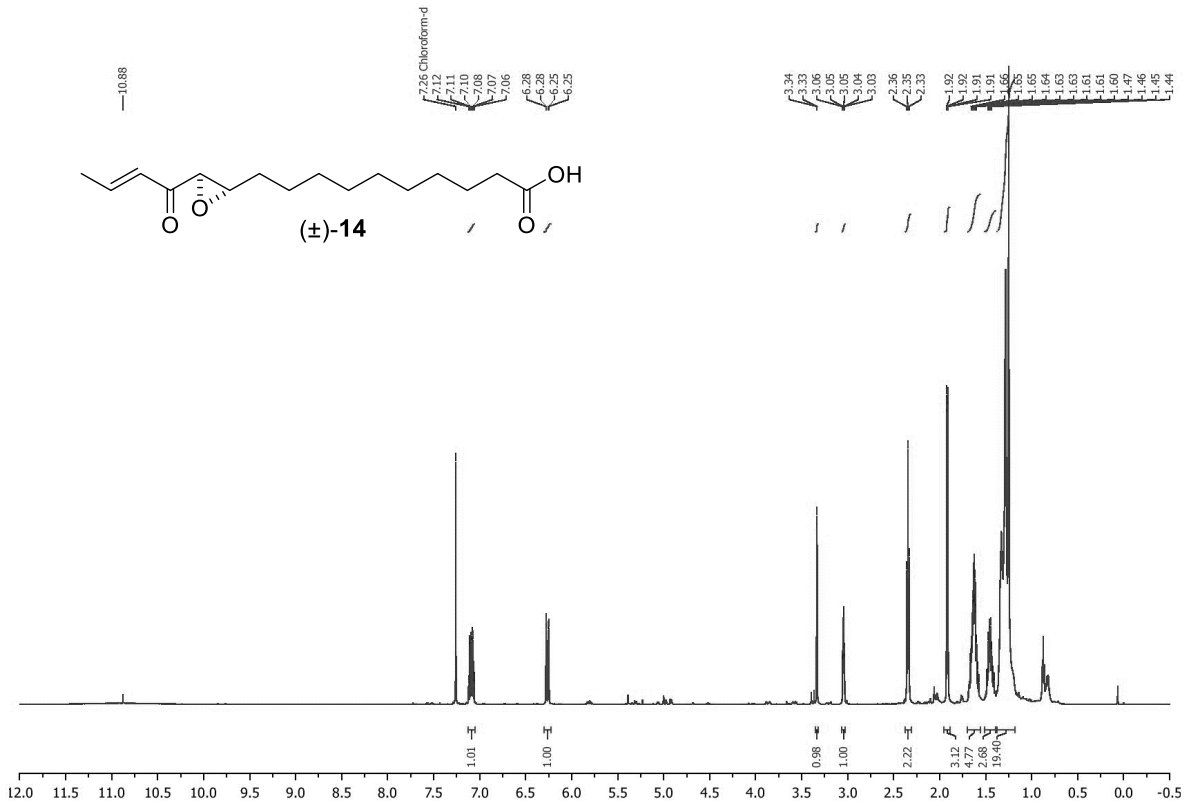
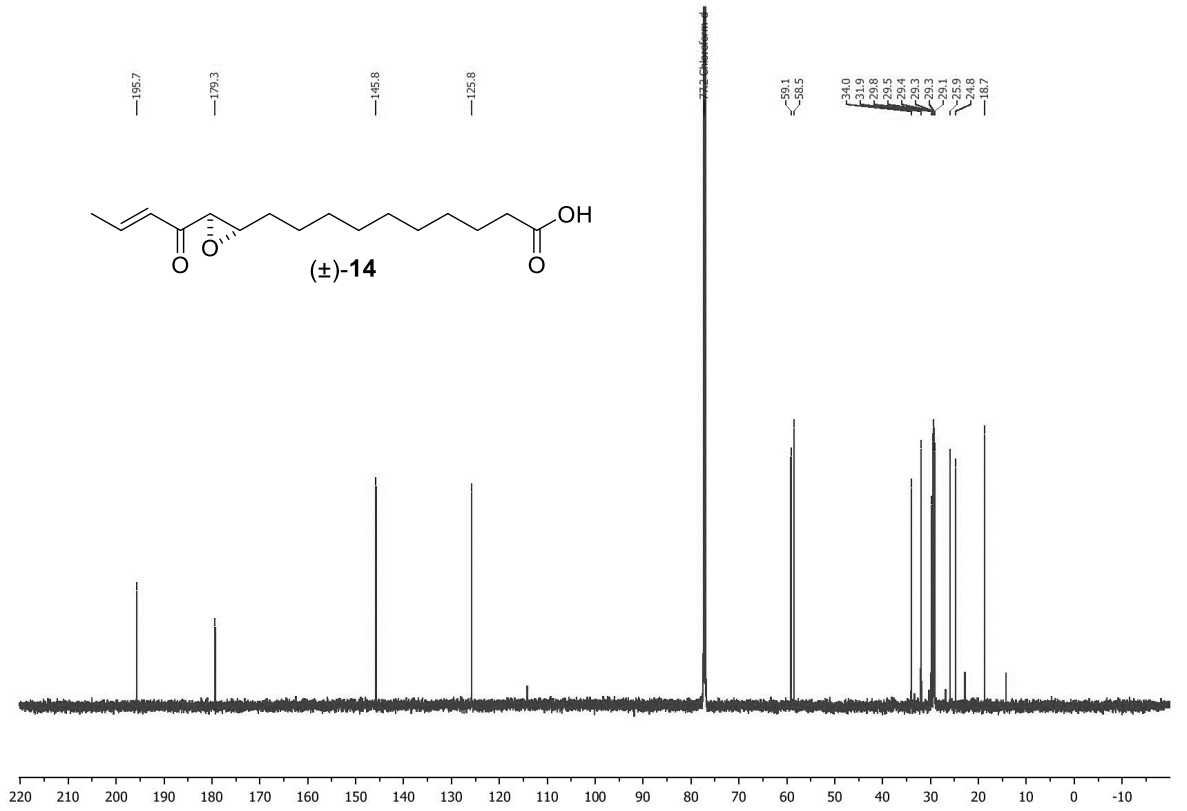
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


(±)-14
OH
O
O
O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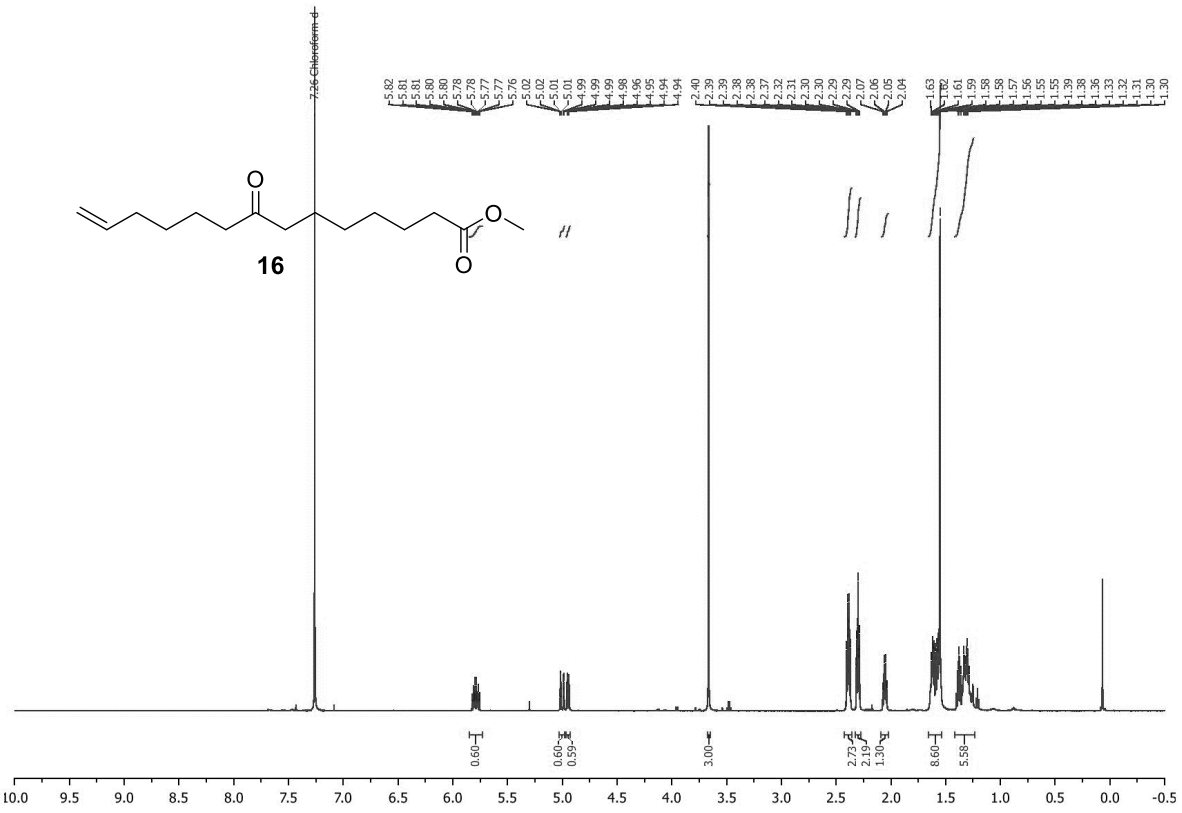
O
O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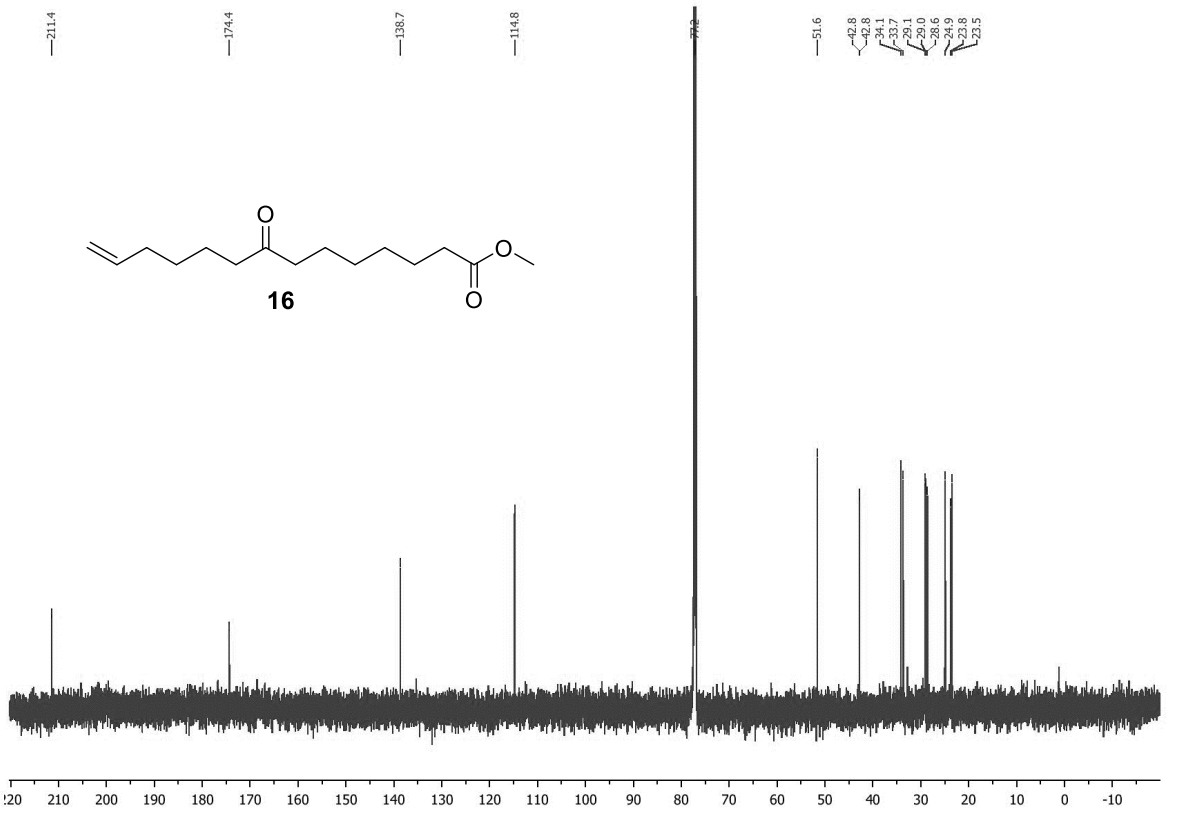
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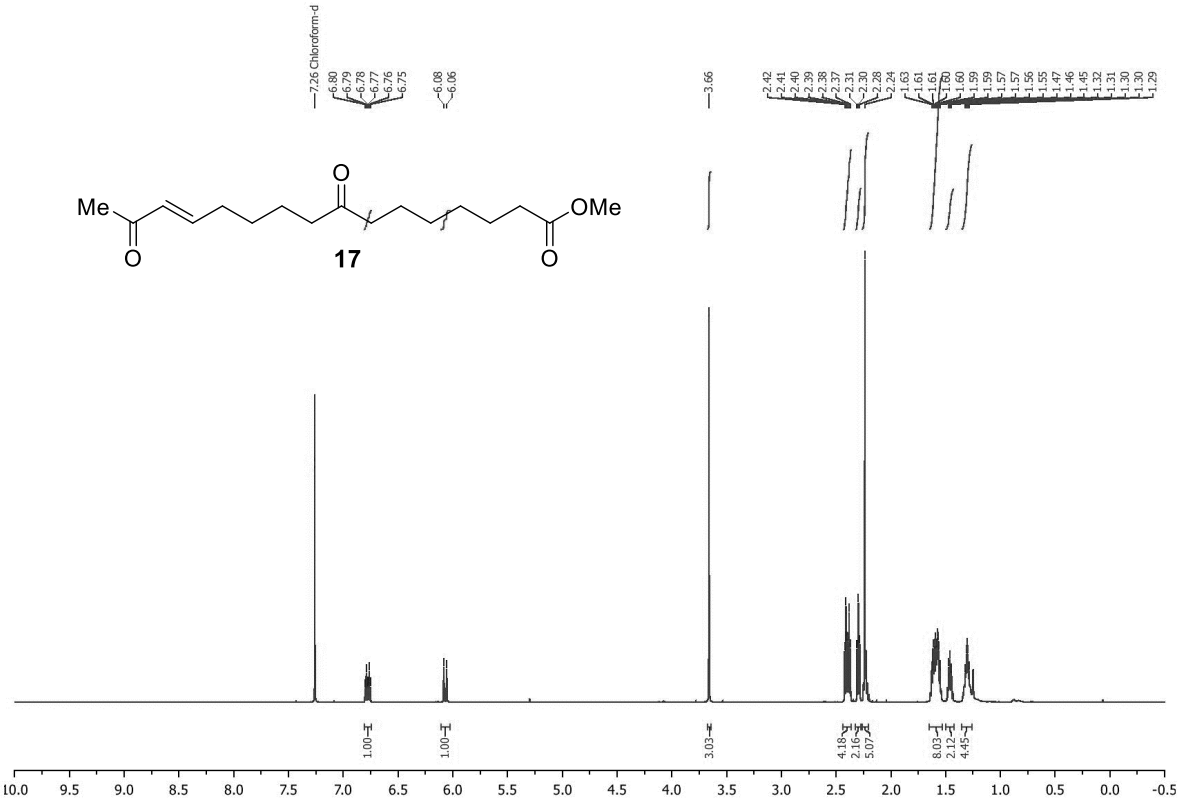
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6.80
6.79
6.78
6.77
6.76
6.75
6.08
6.06
3.66
2.42
2.41
2.40
2.39
2.38
2.37
2.31
2.30
2.28
2.24
1.63
1.61
1.61
1.60
1.60
1.59
1.59
1.57
1.57
1.56
1.55
1.47
1.46
1.45
1.32
1.31
1.30
1.30
1.29
Me
O
O
OMe
O
17
1.00
1.00
3.03
4.18
2.16
5.07
8.03
2.12
4.45
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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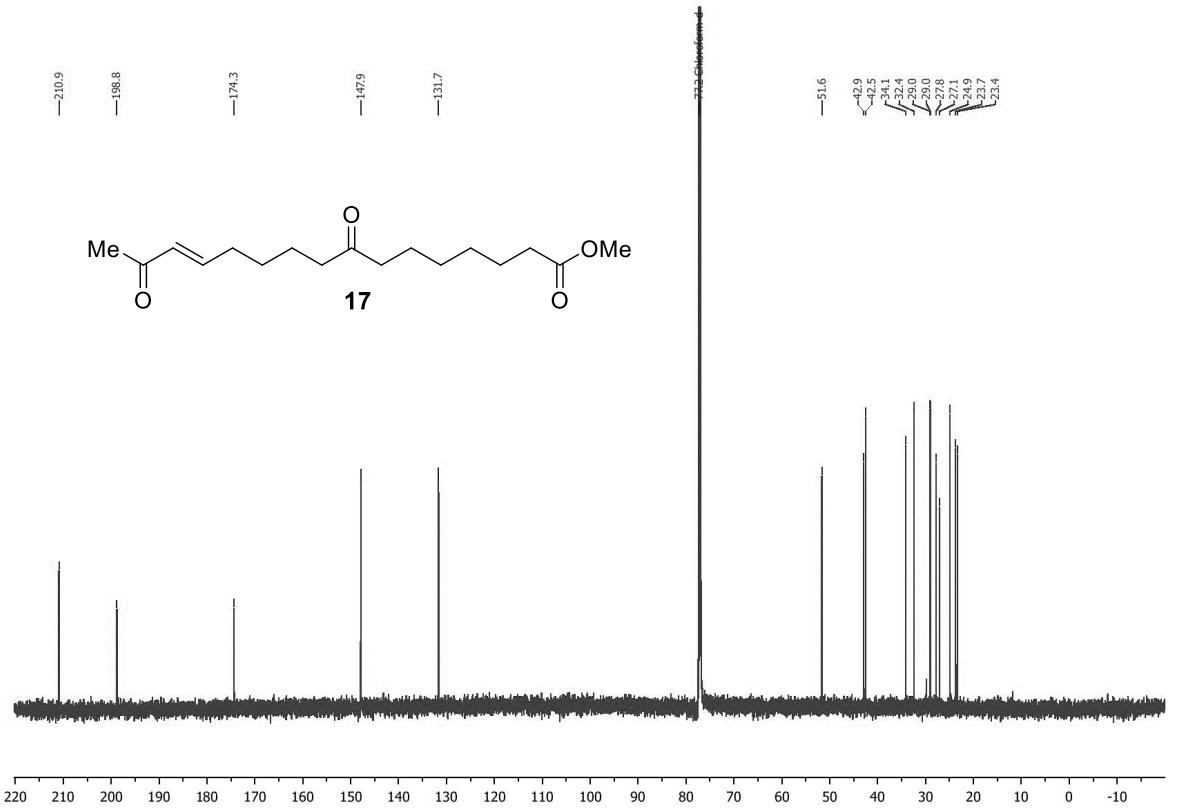
0.0
-0.5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198.8
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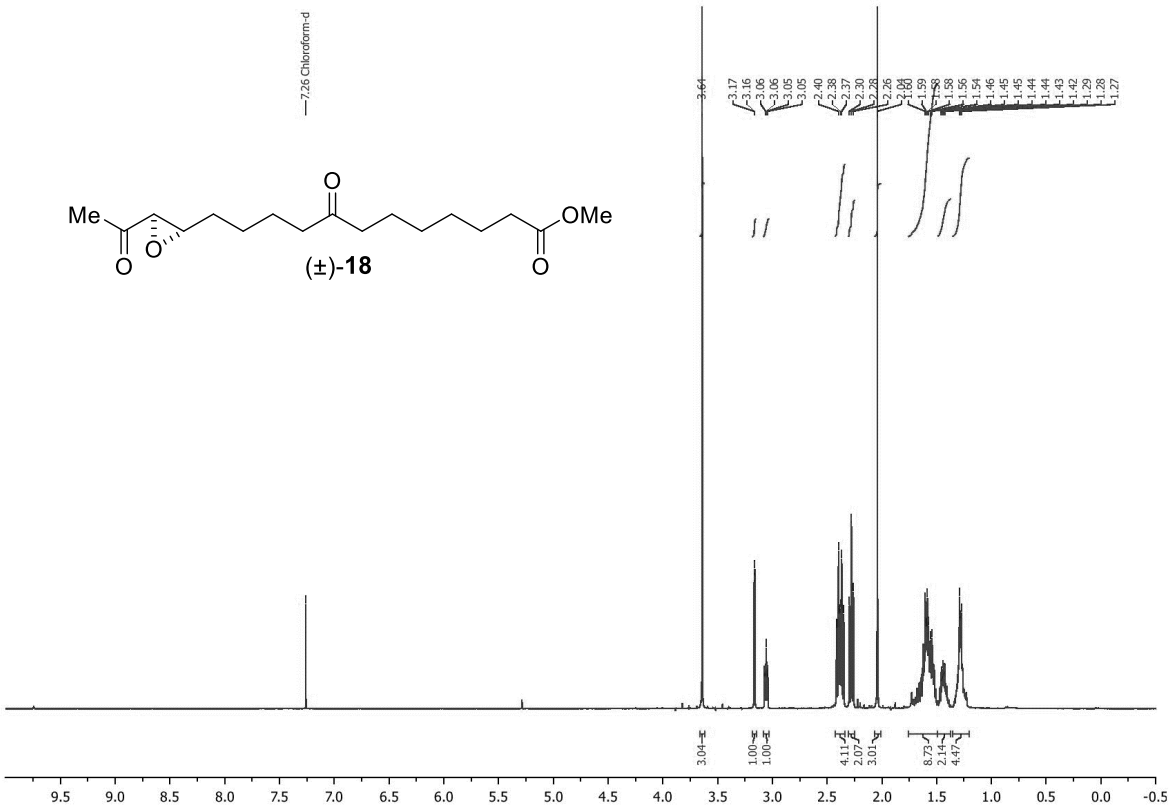
147.9
131.7
77.3 Chloroform-d
51.6
42.9
42.5
34.1
32.4
29.0
29.0
27.8
27.1
24.9
23.7
23.4
Me
O
O
OMe
O
17
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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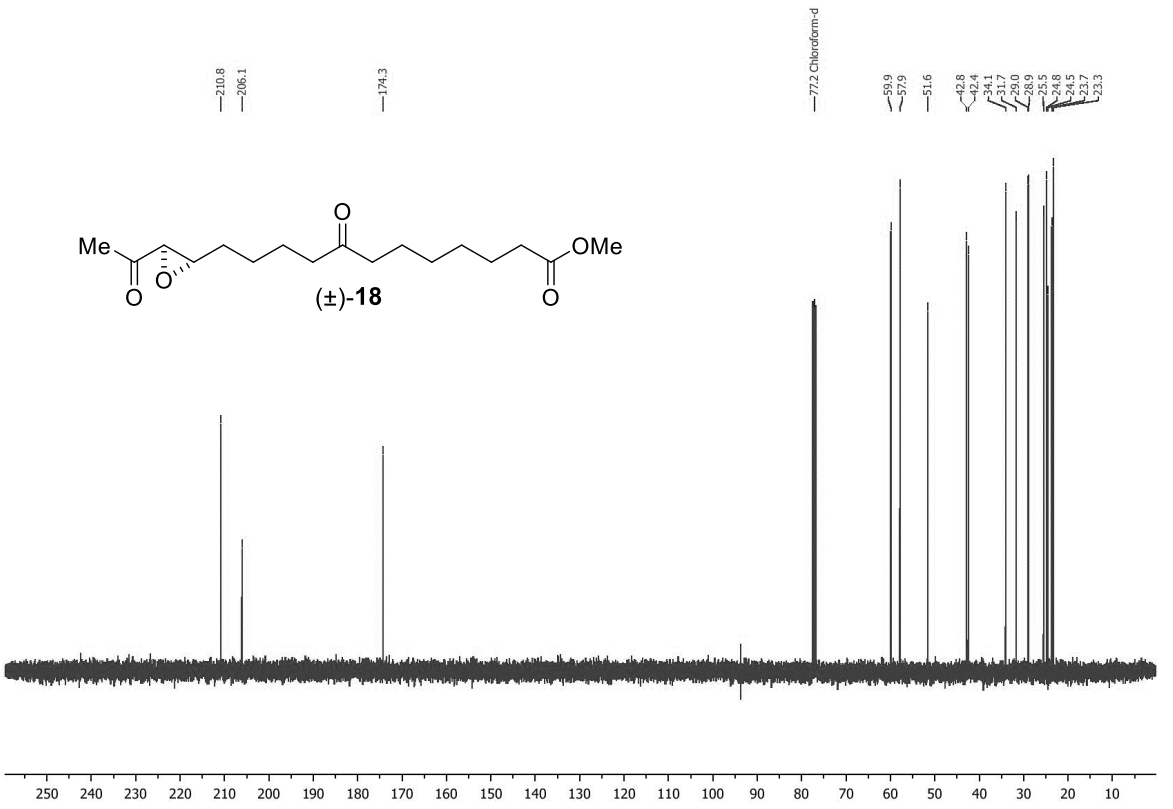
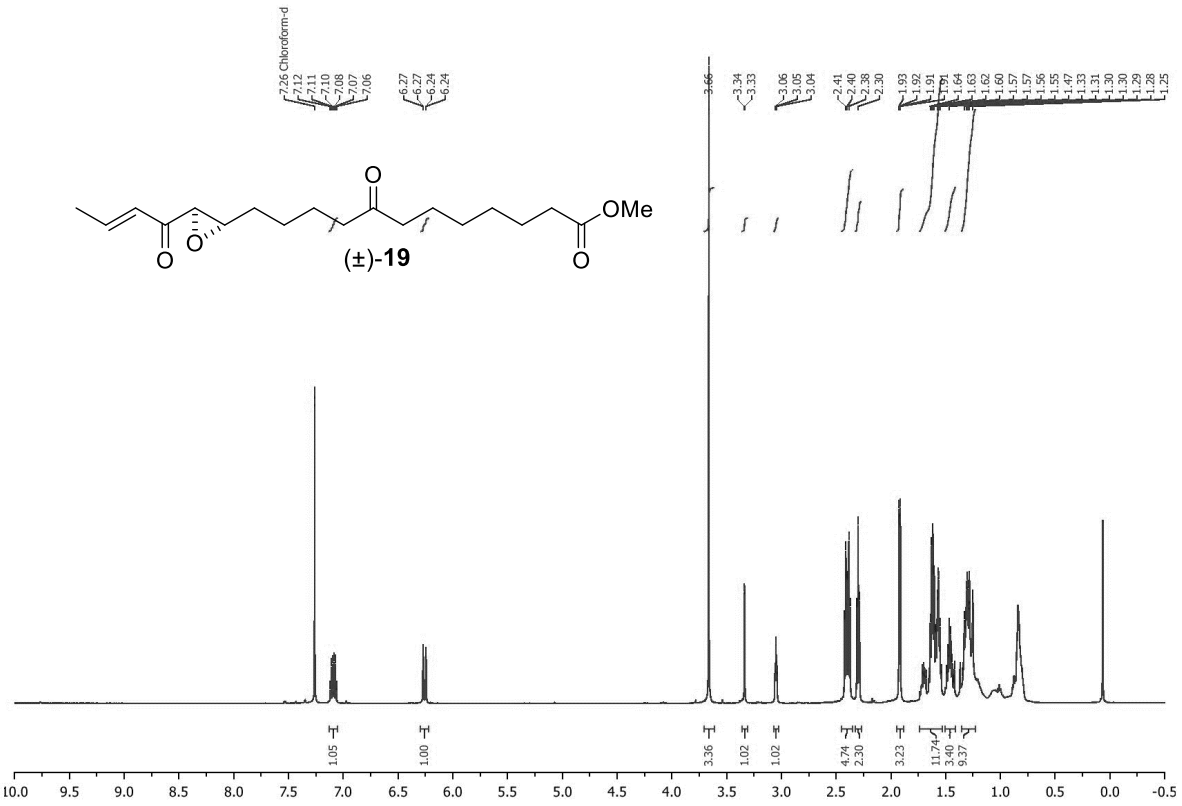
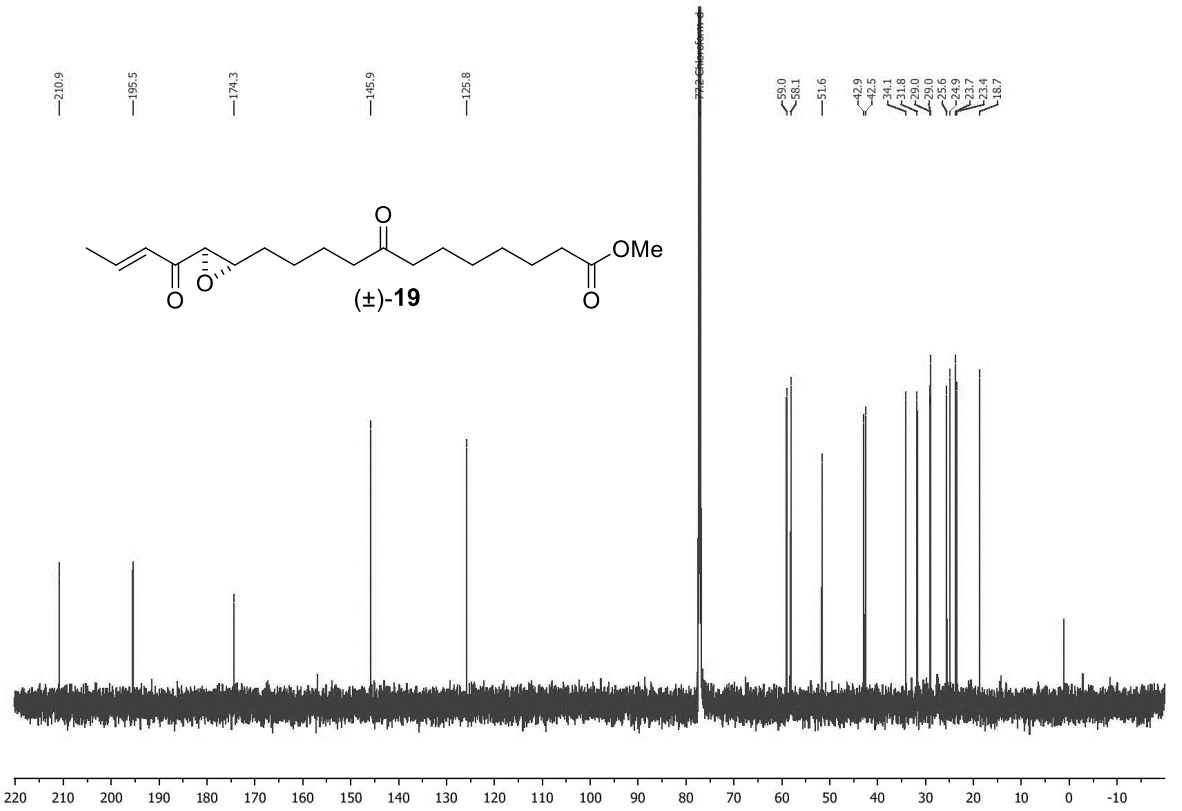
3.06
3.05
3.05
2.40
2.38
2.37
2.30
2.28
2.26
2.04
1.60
1.59
1.58
1.58
1.56
1.54
1.46
1.45
1.45
1.44
1.44
1.43
1.42
1.29
1.28
1.27
Me
O
O
O
O
OMe
(±)-18
3.04
1.00
1.00
4.11
2.07
3.01
8.73
2.14
4.47
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


210.8
206.1
174.3
77.2 Chloroform-d
59.9
57.9
51.6
42.8
42.4
34.1
31.7
29.0
28.9
25.5
24.8
24.5
23.7
23.3
Me
O
O
O
O
OMe
(±)-18
250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


7.26 Chloroform-d
7.12
7.11
7.10
7.08
7.07
7.06
6.27
6.27
6.24
6.24
3.66
3.34
3.33
3.06
3.05
3.04
2.41
2.40
2.38
2.30
1.93
1.92
1.91
1.91
1.64
1.63
1.62
1.60
1.57
1.57
1.56
1.55
1.47
1.33
1.31
1.30
1.30
1.29
1.28
1.25
O
O
O
OMe
O
(±)-19
1.05
1.00
3.36
1.02
1.02
4.74
2.30
3.23
11.74
3.40
9.37
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


210.9
195.5
174.3
145.9
125.8
77.3 Chloroform-d
59.0
58.1
51.6
42.9
42.5
34.1
31.8
29.0
28.0
25.6
24.9
23.7
23.4
18.7
O
O
O
OMe
O
(±)-19
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10